National Aeronautics and
Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

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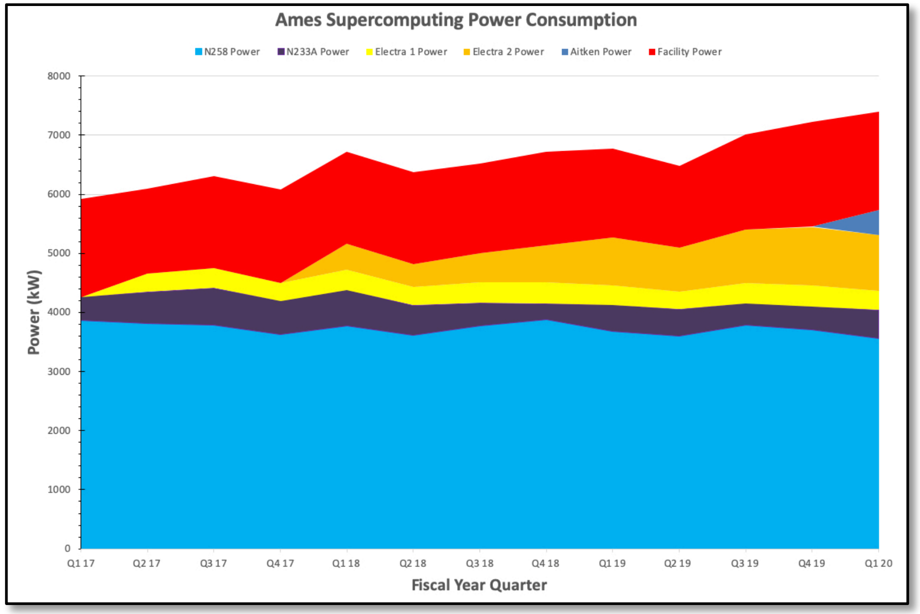
Ames Supercomputing PUE Rating Trending Lower

- The Ames supercomputing Power Usage Effectiveness (PUE) for the first quarter of FY20 was 1.29; and the rolling annual PUE for January through December 2019 was 1.30.
  - PUE, an established metric for computer center power efficiency, is calculated as the (Total Facility Power) ÷ (IT Systems Power).
  - In comparison, reported averages for data centers around the world range from 1.8–2.5 PUE and the average for other NASA data centers is approximately 1.9.

Data Center	FY20 Q1 Oct-Dec 2019	Annual Jan -Dec 2019
N258	1.39	1.37
N233A	1.41	1.49
Electra 1	1.025	1.023
Electra 2	1.040	1.048
Electra combined	1.036	1.042
Aitken	1.053	-
Ames Supercomputing (average total power)	1.29 (7.40MW)	1.30 (7.03MW)

- The Ames supercomputing 7.40-megawatt (MW) average power draw increased 1.5 MW over the last three years while holding the NAS facility average power (non-compute) constant at 1.6 MW.
  - The addition of Electra and Aitken into low PUE facilities will save $400,000 per year in energy costs.

IMPACT: The energy savings provided by low-PUE facilities allows for more HECC funds to be spent on computing and storage resources.



Computing power consumption at NASA's Ames Research Center increased 35% in the last three years, yet the NASA Advanced Supercomputing facility power consumption has remained fixed.

Aitken Module Receives Seismic Improvements

- The module housing the Aitken supercomputer recently received new flexible pipe fittings and pipe stands to improve the capability to operate during and after an earthquake.
- The piping is part of the cooling water infrastructure that circulates water between the Aitken system and the cooling towers.
  - The cooling water infrastructure is vital to the operation of Aitken. Without water flow, the supercomputer is not operable.
- Module suppliers HPE and Schneider Electric conducted a structural analysis of the piping-module interface and incorporated flexible fittings from Metroflex with new pipe stands to support the fittings. The resulting design reduces stress on the module walls and pipe flanges.
  - Aitken was in dedicated time January 27–30 for the upgrade.
  - The Metroflex fittings were installed in both water entry/exit locations into the module and on the water entry into each cooling tower.
- The incorporation of the seismic upgrades improves the availability of the Aitken supercomputer to users, even in the event of natural disasters.

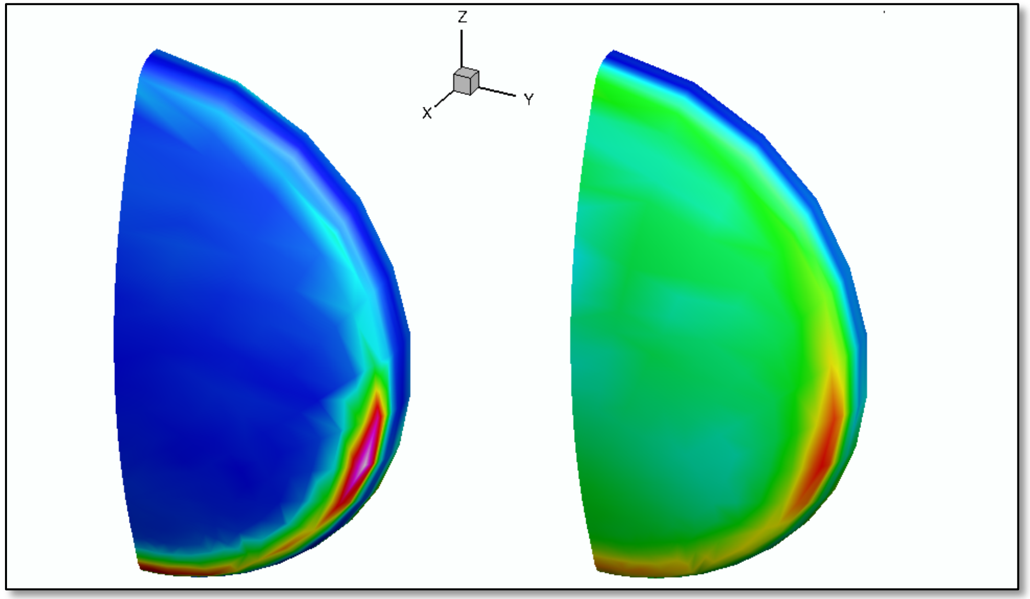
IMPACT: Maintaining a robust cooling system is crucial to the continuous operation of supercomputing capabilities for HECC users.

Newly installed Metroflex fittings and pipe stands on the 6-inch water lines run into the Aitken module. *Chris Tanner*

Monitoring of System Components Leads to Substantial Improvements for Two Applications

- HECC's Application Performance and Productivity (APP) team achieved big performance improvements in two applications that were initially identified by system monitoring as needing investigation.
- APP's proactive monitoring of CPU power usage, looking for load imbalance between the two sockets of a node, identified a climate model application used for analyzing New Horizons data as needing further attention. After contacting the user to explain the situation and to get cooperation, they analyzed the workflow and found a more efficient approach to pack the work onto nodes. The result was a reduction of SBU usage to 6% of what it had been—effectively, a 17-fold improvement.
- Monitoring of Lustre filesystem activity identified inefficient I/O patterns in a heat shield reliability simulation code. APP analyzed the workflow to determine a more efficient approach that reduced the overall time-to-solution by a factor of five—from 10 days to 2 days—by almost eliminating the dependence on Lustre. Now, other users of the filesystem also benefit from fewer I/O requests from that application.

IMPACT: Ongoing performance monitoring of system components, such as compute and storage resources, enables HECC to improve both user turnaround times and overall system utilization.



The left image shows the reliability of the spacecraft heat shield for guided entry of Orion against over-temperature of its bond to the substructure. The right image shows the average amount of Avcoat material that will remain. *Steve Sepka, NASA/Ames*

Tools Team Upgrades LAMS Database to Red Hat 7

- The HECC Tools Team completed the upgrade of the LAMS database system to Red Hat Enterprise Linux 7.
  - The LAMS database is one of the key infrastructure components for managing all HECC user accounts and allocations.
- Key activities that were completed in order to achieve this milestone include:
  - Migrated from the MySQL 5.1 database to MariaDB 5.5 and verified the accounts, triggers, and functions; and created missing database procedures.
  - Created a new database connection to the MariaDb database from Oracle acctdb and the Remedy database to sync the user, group, host, and allocation information.
  - Modified and tested all the cronjobs running from the LAMS database to remote systems. Verified that scripts are correctly pushing out the necessary files from LAMS.
  - Verified and installed all the necessary Perl modules needed by the cronjobs scripts.
  - Verified the accounts database connection and data pipeline between the account request form and the LAMS database.

IMPACT: Upgrades to the LAMS database are essential to ensuring accurate, efficient management of user accounts and allocations on all HECC resources.

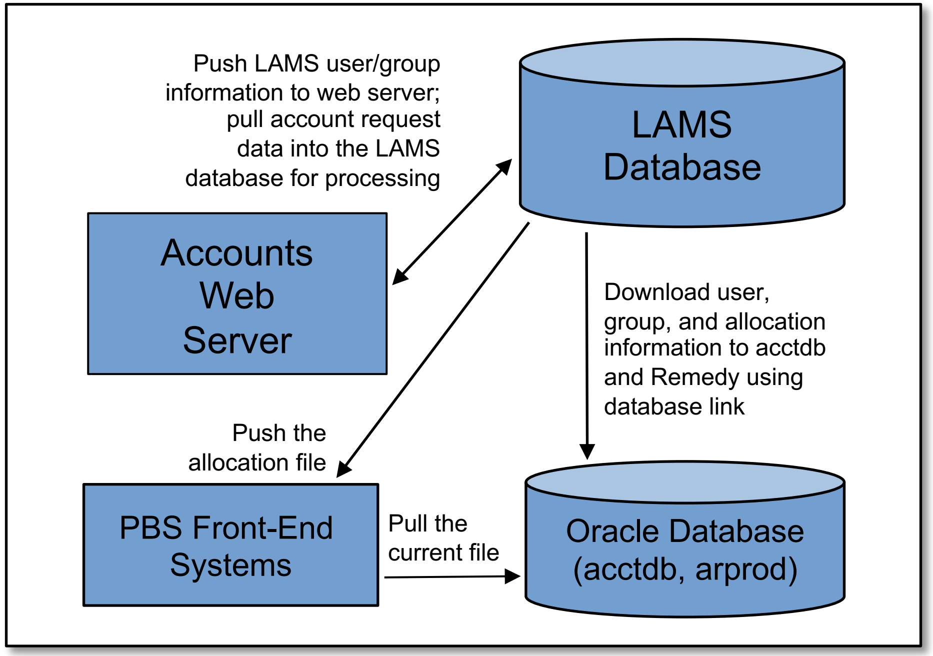


Chart showing the flow of user information for the HECC account management process.

User Services Releases Survey Results, Recommendations

- The 2019 survey results and recommendations were released to HECC management. The survey identifies areas for improvement, year-to-year trends, and user satisfaction across each of the project's service areas. This information is then used to provide recommendations and actions completed to date.
- User Support staff continue to be HECC's strong suit, receiving high praise from users for both quality and timeliness of work.
- Other areas of high satisfaction included: compute power, system reliability, and the availability and completeness of training materials and the Knowledge Base.
- Four main areas of opportunity for improvement were identified: software packages and licenses, allocation services and availability of resources, communication with users, and training materials.
- Recommendations included a revamp of HECC's user communications plan, development of short video tutorials for basic tasks, and a review of the allocation process, among other items.

IMPACT: Regular user survey results are used to generate recommendations and provide actions-to-date to inform management decisions. These recommendations align with HECC user feedback on what areas need the most improvement, as well as trends identified in the survey data.

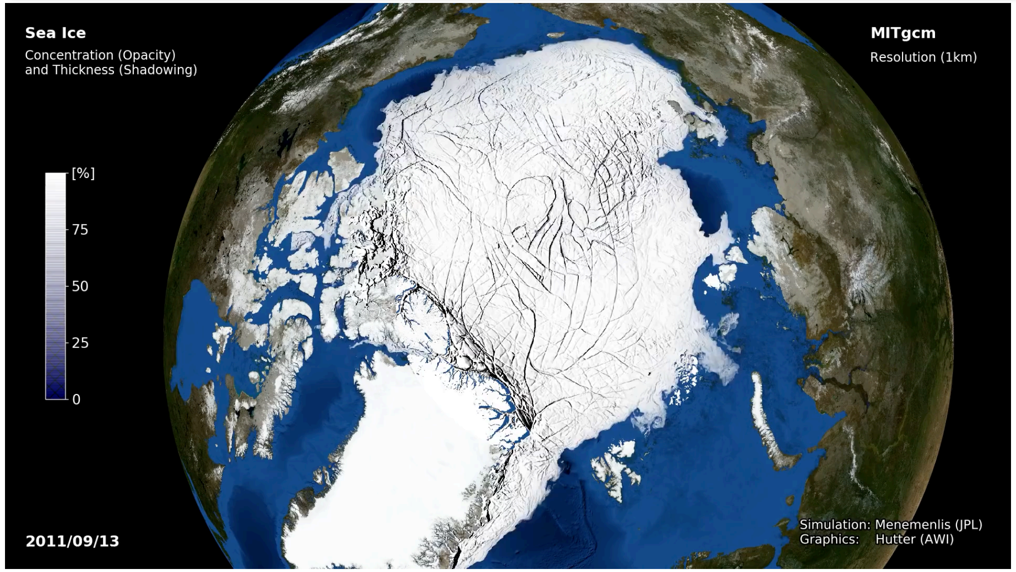
Word cloud generated from user responses to "What aspects of NAS Services are outstanding?"

Realistic Simulations of the Coupled Atmosphere-Ocean-Ice System *

- Earth science researchers are successfully running groundbreaking coupled ocean-atmosphere simulations, using two flagship data-assimilating NASA models, in order to accurately represent and understand coupled air-sea exchange processes.
  - The Goddard Earth Observing System (GEOS), which is used for global cloud-resolving simulations with horizontal grid spacing as small as 1.5 kilometers (km).
  - The Estimating the Circulation and Climate of the Ocean (ECCO) model, which is used for global-ocean, submesoscale and internal-wave-admitting simulations with horizontal grid spacing as small as 1–2 km.
- Initial analysis of the coupled-model output revealed three-to-six-day oscillations of sea surface temperatures and surface wind anomalies—a phenomenon appearing in observational records and reanalyses, but previously unseen in ocean-only simulations.
- These simulations are also used to guide the utilization of existing satellite observations and development of new instruments.
- The simulations are available to the scientific community on NAS and NCCS data portals.

** HECC provided supercomputing resources and services in support of this work.*

IMPACT: NASA supercomputing resources are revolutionizing Earth science studies by enabling increasingly realistic simulations of the coupled ice-ocean-atmosphere system that are shared with and used by the scientific community.



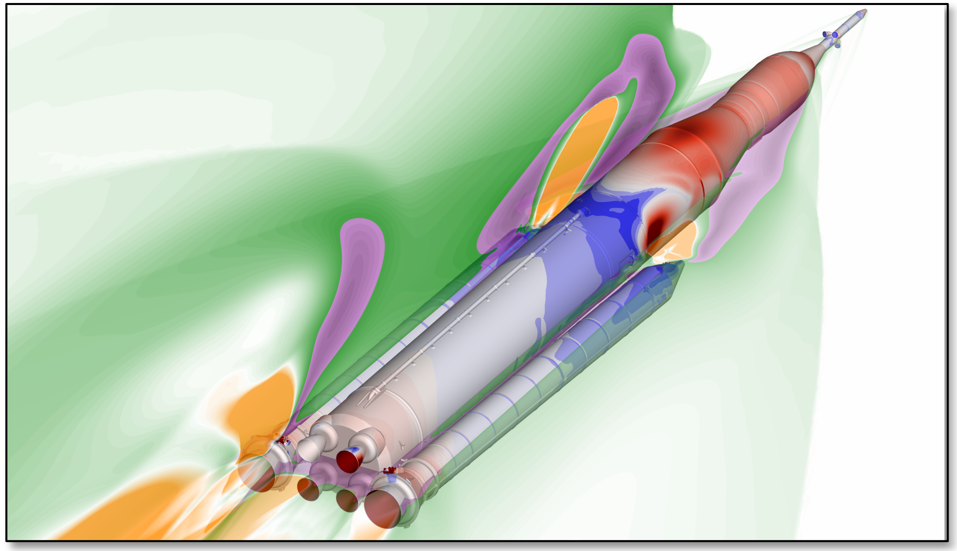
Video showing Arctic sea ice concentration and thickness from an internal-wave-admitting Estimating the Circulation and Climate of the Ocean (ECCO) simulation. The small-scale deformation of the ice causes the sea ice cover to be divided into several floes separated by strips of open ocean called "leads." *Dimitris Menemenlis, NASA/JPL; Nils Hutter, Alfred-Wegener Institute*

Building Booster Separation Aerodynamic Databases for Artemis II *

- Aerospace engineers at NASA Ames ran computational fluid dynamics (CFD) simulations on the Pleiades and Electra supercomputers to formulate the booster separation databases for NASA's Artemis II flight configuration.
- Created using NASA's FUN3D flow solver, the calculations include the aerodynamic effects of 22 different plumes during the booster separation event and 13 independent variables. Additionally, separate sets of computations were run to simulate possible effects caused by a core-stage engine failure.
- These databases will be used by the Guidance, Navigation, and Control group at NASA Marshall to create dynamic simulations of the booster separation event for Artemis II to ensure the boosters can separate successfully without reconnecting to the core under all possible flight conditions.
- The CFD simulations that construct these databases allow engineers to model flight conditions and complex interactions that are difficult to test in an experimental setting.

** HECC provided supercomputing resources and services in support of this work.*

IMPACT: The results of these simulations, run on HECC resources, will be critical in reducing the risk to the crew of the Artemis II missions during booster separation.



Isometric view of the Artemis II vehicle, simulating the effect of a failure in a core stage engine with the boosters four feet downstream from their original, attached position. Slices of the flow are taken on vehicle centerline and through the left booster's separation motors. The vehicle surface is colored by pressure contours, where blue is low and red is high. The green and orange colors represent low and high Mach numbers, respectively.
Stuart Rogers, Jamie Meeroff, NASA/Ames

HECC Facility Tours in January 2020

- HECC hosted 6 tour groups in November; guests learned about the agency-wide missions being supported by HECC assets and viewed the D-Wave 2000Q quantum system. Visitors this month included:
  - Chris Fall, Director, Office of Science, Department of Energy was briefed by Piyush Mehrotra, Bill Thigpen, and Chris Henze on how NASA supercomputer systems are being used by NASA researchers.
  - A group from Australia's Victorian Space Science Education Centre, representing winners of a Science, Technology, Engineering, and Math and an entrepreneurship competition in Australia; students toured NASA Centers as part of the prize.
  - Chris Schmitt, Congressional Liaison, Navy Office of Legislative Affairs; and Senate Armed Services Committee members Jonathan Epstein and Arun Seraphin, were briefed by Eleanor Rieffel and Piyush Mehrotra on NASA Ames' quantum and supercomputing systems.
  - A group of researchers from Stanford, UC Berkeley, and Lawrence Livermore National Laboratories, hosted by the Ames Early Career Network.
  - Students in the Ames spring internship program.

Darrel Robertson, a research engineer in the NASA Advanced Supercomputing (NAS) Division, briefs students in the NAS facility's quantum computer room. *Gina Morello, NASA/Ames*

Papers

- “**The First Habitable Zone Earth-Sized Planet from TESS: Spitzer Confirms TOI-700 d**,” J. Rodriguez, et al., arXiv:2001.00954 [astro-ph.EP], January 3, 2020. *
  https://arxiv.org/abs/2001.00954
- “**The First Habitable Zone Earth-Sized Planet from TESS. I.: Validation of the TOI-700 System**,” E. Gilbert, et al., arXiv:2001.00952 [astro-ph.EP], January 3, 2020. *
  https://arxiv.org/abs/2001.00952
- “**Thermosphere-Ionosphere Modeling with Forecastable Inputs: Case Study of the June 2012 High-Speed Stream Geomagnetic Storm**” X. Meng, et al., Space Weather, vol. 18, issue 2, January 5, 2020. *
  https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2019SW002352
- **AIAA SciTech 2020 Forum**, Orlando, FL, January 6-10, 2020.
  – “**Direct Numerical Simulations of Acoustic Disturbances in Various Rectangular Nozzle Configurations**,” N. Hildebrand, M. Choudhari, L. Duan. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2020-0587
  – “**Unstructured Grid Development for the Space Launch System Liftoff and Transition Lineloads Computational Analysis**,” N. Ratnayake, S. Krist, F. Ghaffari, V. Ahmed. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2020-0672

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- **AIAA SciTech 2020 Forum (cont.)**
  - “**Pterodactyl: Aerodynamic and Aeroheating Database Development for Integrated Control Design of a Mechanically Developed Entry Vehicle**,” B. Nikaido, Z. Hays, B. Reddish. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2020-1010
- “**Energetic Submesoscale Dynamics in the Ocean Interior**,” L. Siegelman, Journal of Physical Oceanography, published online January 9, 2020. *
  https://journals.ametsoc.org/doi/abs/10.1175/JPO-D-19-0253.1
- “**Age Dating of an Early Milky Way Merger via Asteroseismology of the Naked-Eye Star *ν* Indi**,” W. Chaplin, et al., Nature Astronomy: Letters, January 13, 2020. *
  https://www.nature.com/articles/s41550-019-0975-9
- “**Magnetohydrodynamic with Embedded Particle-in-Cell Simulation of the Geospace Environment Modeling Dayside Kinetic Processes Challenge Event**,” Y. Chen, et al., arXiv:2001.04563 [physics.space-ph], January 13, 2020. *
  https://arxiv.org/abs/2001.04563
- “**Interpreting Observations of Absorption Lines in the Circumgalactic Medium with a Turbulent Medium**,” E. Buie II, M. Fumagalli, E. Scannapeico, arXiv:2001.04965 [astro-ph.GA], January 14, 2020. *
  https://arxiv.org/abs/2001.04965

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- "**Electron Acceleration from Expanding Magnetic Vortices During Reconnection with a Guide Field**," H. Che, G. Zank, The Astrophysical Journal, vol. 889, no. 1, January 20, 2020. *
https://iopscience.iop.org/article/10.3847/1538-4357/ab5d3b/meta
- "**Figuring Out Gas & Galaxies in Enzo (FOGGIE). III. The Mocky Way: Investigating Biases in Observing the Milky Way's Circumgalactic Medium**," Y. Zheng, et al., arXiv:2001.07736 [astro-ph.GA], January 21, 2020. *
https://arxiv.org/abs/2001.07736
- "**A Hot Terrestrial Planet Orbiting the Bright M Dwarf L 168-9 Unveiled by TESS**," N. Astrudillo-Defru, et al., arXiv:2001.09175 [astro-ph.EP], January 24, 2020. *
https://arxiv.org/abs/2001.09175
- "**A Fully Kinetic Perspective of Electron Acceleration Around a Weakly Outgassing Comet**," A. Divin, et al., The Astrophysical Journal Letters, vol. 889, no. 2, January 29, 2020. *
https://iopscience.iop.org/article/10.3847/2041-8213/ab6662/meta
- "**Rankine-Hugoniot Relations Including Pickup Ions**," M. Gedalin, N. Pogorelov, V. Roytershteyn, The Astrophysical Journal, vol. 889, no. 2, January 30, 2020. *
https://iopscience.iop.org/article/10.3847/1538-4357/ab6660/meta

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Presentations

- **AIAA SciTech 2020 Forum**, Orlando, FL, January, 6–10, 2020.
  - “**Computational Study of NASA’s Quadrotor Urban Air Taxi Concept**,” P. Ventura Diaz, S. Yoon. *
    https://arc.aiaa.org/doi/10.2514/6.2020-0302
  - “**Multigrid Preconditioning for a Space-Time Spectral-Element Discontinuous-Galerkin Solver**,” M. Franiolini, S. Murman. *
    https://arc.aiaa.org/doi/10.2514/6.2020-1314
  - “**Development of Unsteady-PSP Data Processing and Analysis Tools for the NASA Ames Unitary 11ft Wind Tunnel**,” J. Powell, S. Murman, C. Ngo, N. Roozeboom, D. Murakami, J. Baerny, J. Lie.
    https://arc.aiaa.org/doi/10.2514/6.2020-0292
  - “**Considering Deflection Missions for Asteroid Impact Risk**,” C. Rumpf, D. Mathias, L. Wheeler, J. Dotson.
    https://arc.aiaa.org/doi/10.2514/6.2020-0222
  - “**Analysis of Three Multi-Band Models for Radiative Heat Transfer in LTE Air Plasma**,” S. Izquierdo, J. Meurisse, S. Visser, M. Haw, J. Schultz, N. Mansour. *
    https://arc.aiaa.org/doi/10.2514/6.2020-0735
  - “**Preliminary Measurements of the Motion of Arcjet Current Channel Using Inductive Magnetic Probes**,” M. Haw, J. Meurisse, S. Visser, S. Izquierdo, J. Schulz, N. N. Mansour. *
    https://arc.aiaa.org/doi/10.2514/6.2020-0919
  - “**A Numerical Investigation of Parachute Deployment in Supersonic Flow**,” J. Boustani, G. Anugrah, M. Barad, C. Kiris, C. Brehm. *
    https://arc.aiaa.org/doi/10.2514/6.2020-1050

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Presentations (cont.)

- **AIAA SciTech 2020 Forum (cont.)**
  - "**Comparison of Algorithms for High-Order, Metric-Based Mesh Optimization**," D. Sanjaya, K. Fidkowski, S. Murman. *
    https://arc.aiaa.org/doi/10.2514/6.2020-1141
  - "**Reynolds-Averaged Navier-Stokes Computations of the NASA Juncture Flow Model Using FUN3D and OVERFLOW**," C. Rumsey, H. Lee, T. Pulliam. *
    https://arc.aiaa.org/doi/10.2514/6.2020-1304
  - "**Computational Simulations of a Mach 0.745 \\Transonic Truss-Braced Wing Design**," D. Maldonado, S. Viken, J. Housman, C. Hunter, J. Duensing, N. Frink, et al. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2020-1649
  - "**High-Fidelity Numerical Analysis of Arc-Jet Aerothermal Environments**," P. Ventura Diaz, A. Parente, J. Meurisse, S. Yoon, N. N. Mansour. *
    https://arc.aiaa.org/doi/10.2514/6.2020-1710
  - "**Effects of Spatial Resolution on Retropropulsion Aerodynamics in an Atmospheric Environment**," A. Korzun, E. Nielsen, A. Walden, W. Jones, J. Carlson, P. Moran, C. Henze, T. Sandstrom. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2020-1749

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Presentations (cont.)

- **AIAA Sonic Boom Prediction Workshop**, Orlando, FL, January 6–10, 2020.
  - “**sBoom Propagation for the Third AIAA Sonic Boom Prediction Workshop**,” M. Aftosmis, W. Spurlock. *
    https://ntrs.nasa.gov/archive/nasa/casi.ntrs.nasa.gov/20200000443.pdf (PDF 2.6 MB)
  - “**LAVA Results for SBPW3**,” J. Jensen, J. Duensing, M. Piotrowski, J. Housman, D. Maldonado, C. Kiris. *
    https://ntrs.nasa.gov/archive/nasa/casi.ntrs.nasa.gov/20200000441.pdf (PDF 1.2 MB)
  - “**Cartesian Mesh Simulations for the 3rd AIAA Sonic Boom Prediction Workshop**,” W. Spurlock, M. Aftosmis. M. Nemec. *
    https://ntrs.nasa.gov/archive/nasa/casi.ntrs.nasa.gov/20200000440.pdf (PDF 1.2 MB)

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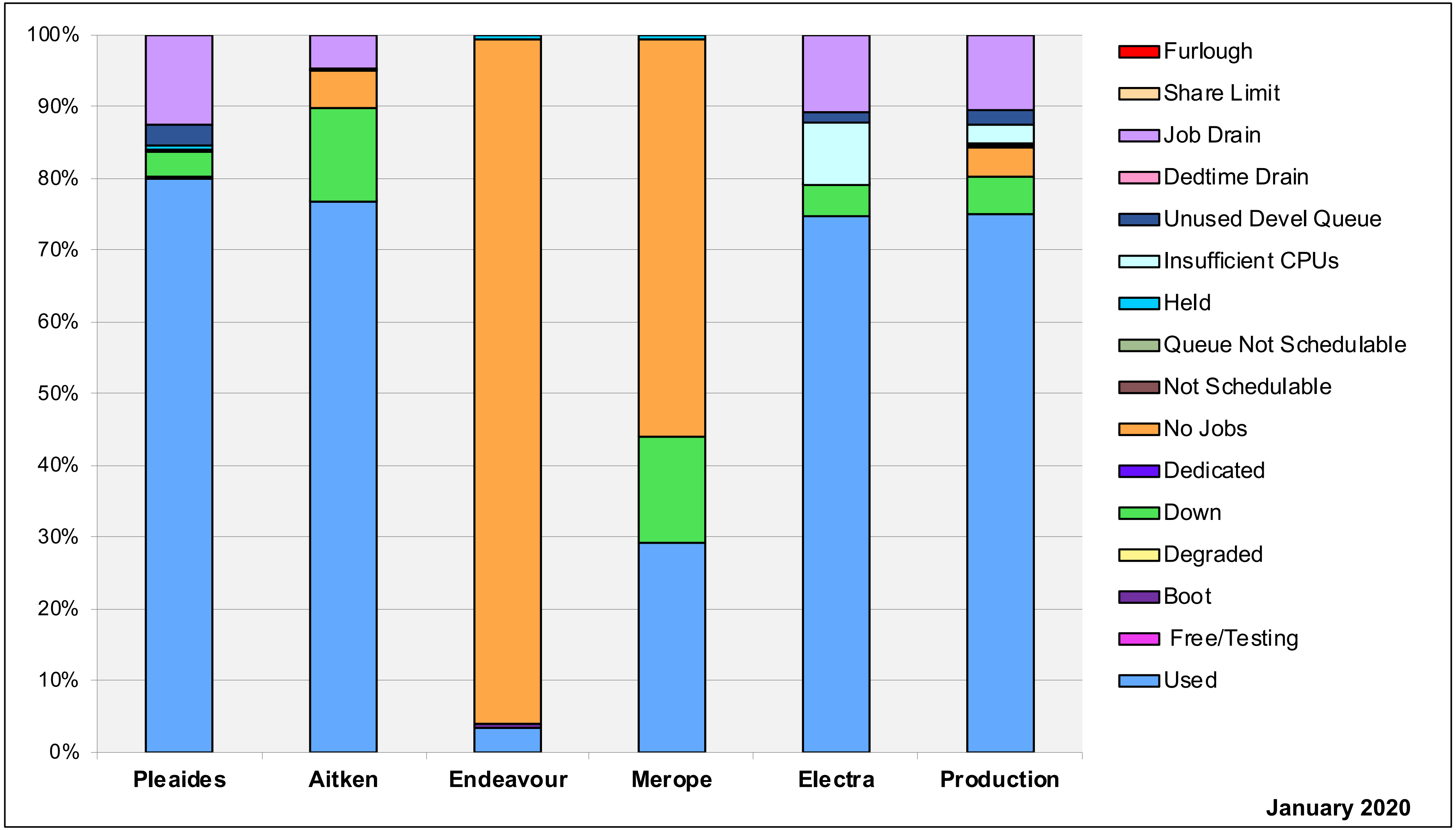
News and Events

- **Simulations Reveal Galaxy Clusters Details**, *Texas Advanced Computing Center*, January 23, 2020—Inspired by the science fiction of the spacefaring Romulans of Star Trek, astrophysicists have developed cosmological computer simulations called RomulusC, and run them on some of the most powerful supercomputers in the U.S., including NASA's Pleiades supercomputer. With a focus on black hole physics, RomulusC has produced some of the highest resolution simulations ever of galaxy clusters, which can contain hundreds or even thousands of galaxies.
  https://www.tacc.utexas.edu/-/simulations-reveal-galaxy-clusters-details
  - **Supercomputer Simulations Reveal Details of Galaxy Clusters**, *HPCwire*, January 27, 2020
    https://www.hpcwire.com/off-the-wire/supercomputer-simulations-reveal-details-of-galaxy-clusters/

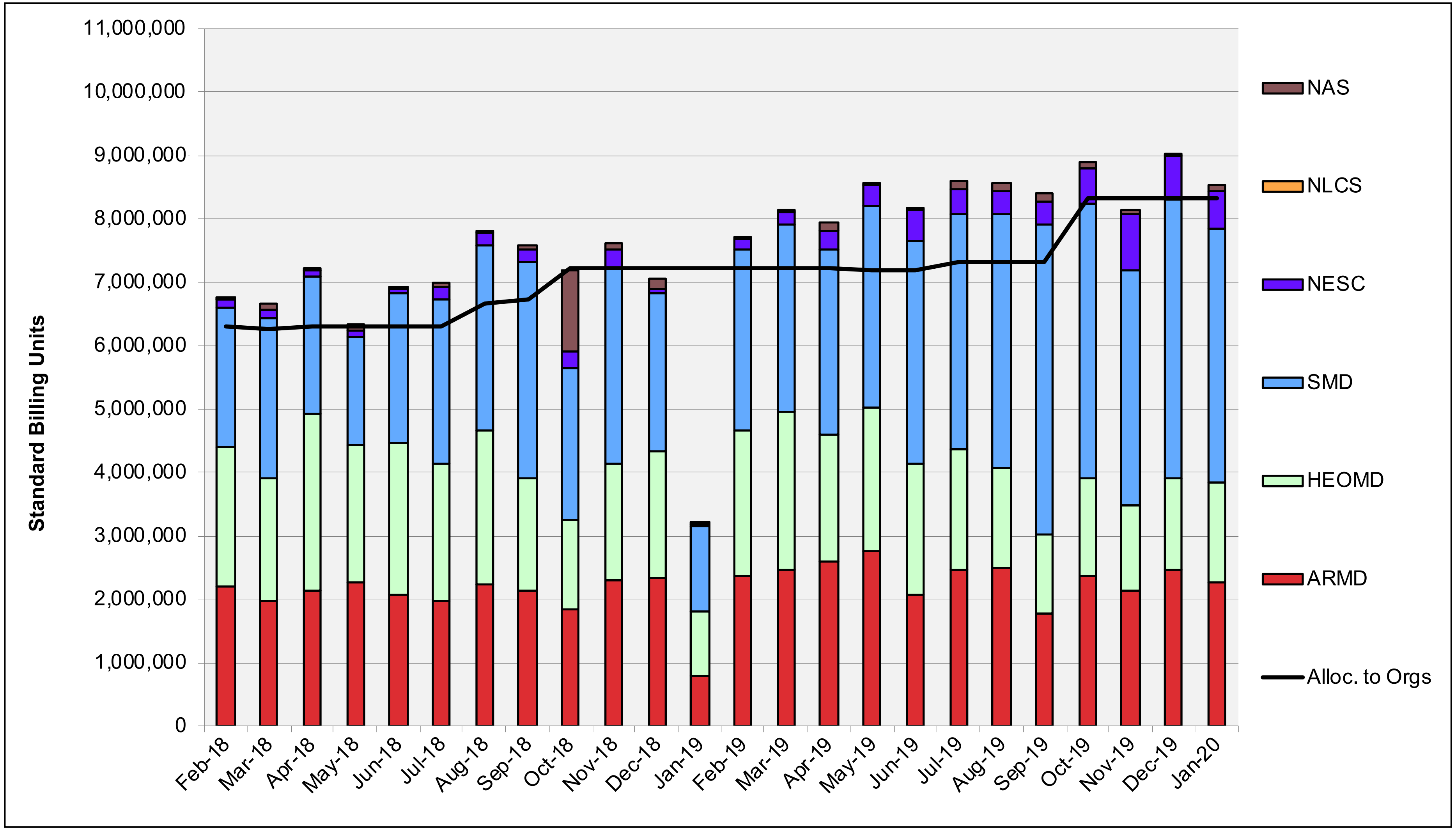
News and Events: Social Media

- **Coverage of NAS Stories**
  - Orion Launch Simulation named one of 2019's most beautiful science GIFs
    - NAS: Twitter 25 retweets, 137 favorites
  - Throwback NAS Feature Stories
    - Hot Jupiter Simulations, NAS: Twitter 1 retweet, 9 likes
    - SC19 Wrap-up, NAS: Twitter 2 retweets, 5 likes
    - Asteroid Impact Simulations, NAS: Twitter 3 retweets, 6 likes
  - Supercomputer Simulations Reveal Details of Galaxy Clusters
    - NAS : Twitter 1 share, 5 retweets, 8 favorites
    - HPCwire: Twitter 1 retweet, 4 likes

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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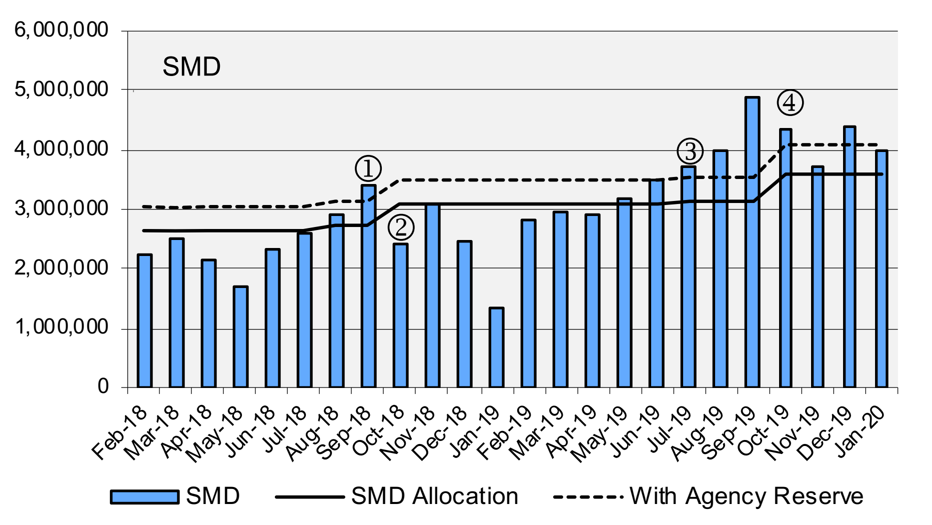
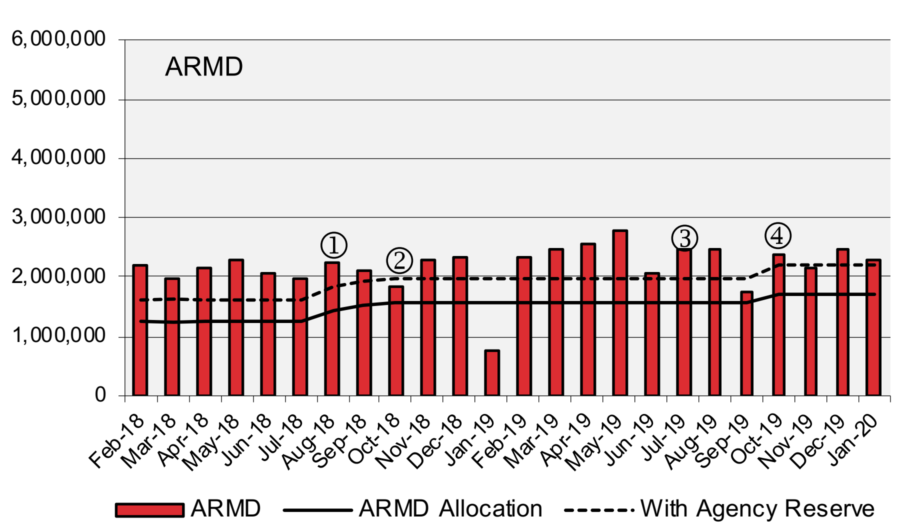
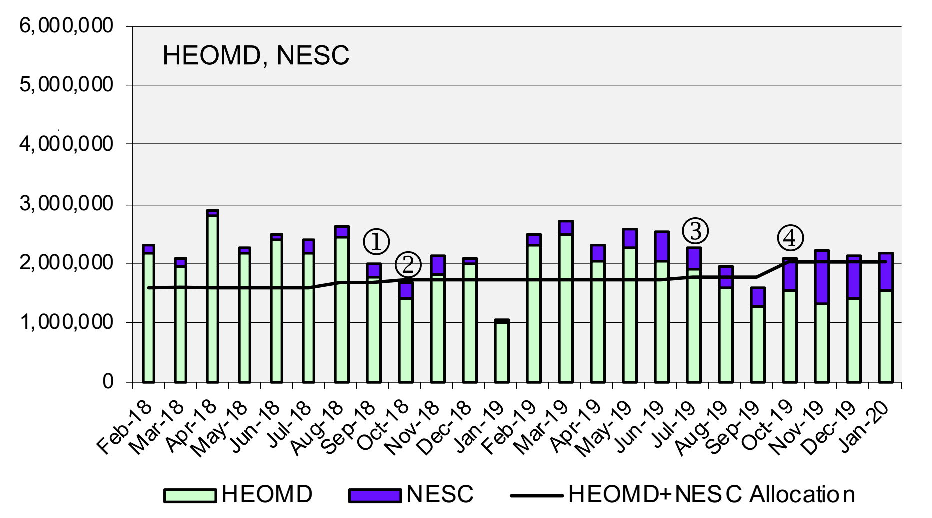






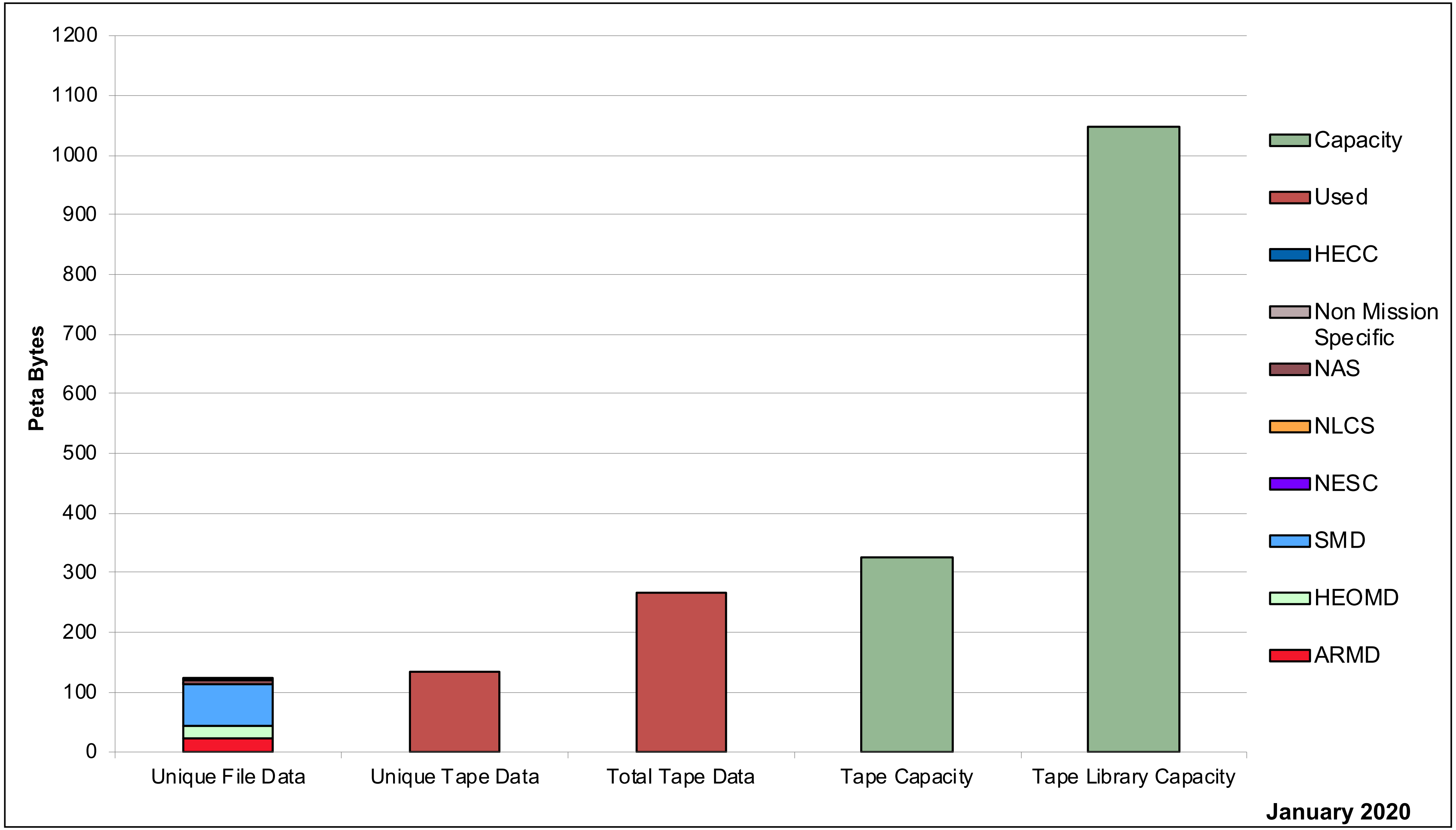
① 4 Skylake E cells (16 D Rack Equivalence) added to Electra

② 2 Skylake E cells (8 D Rack Equivalence) added to Electra; 1 rack is dedicated to ARMD

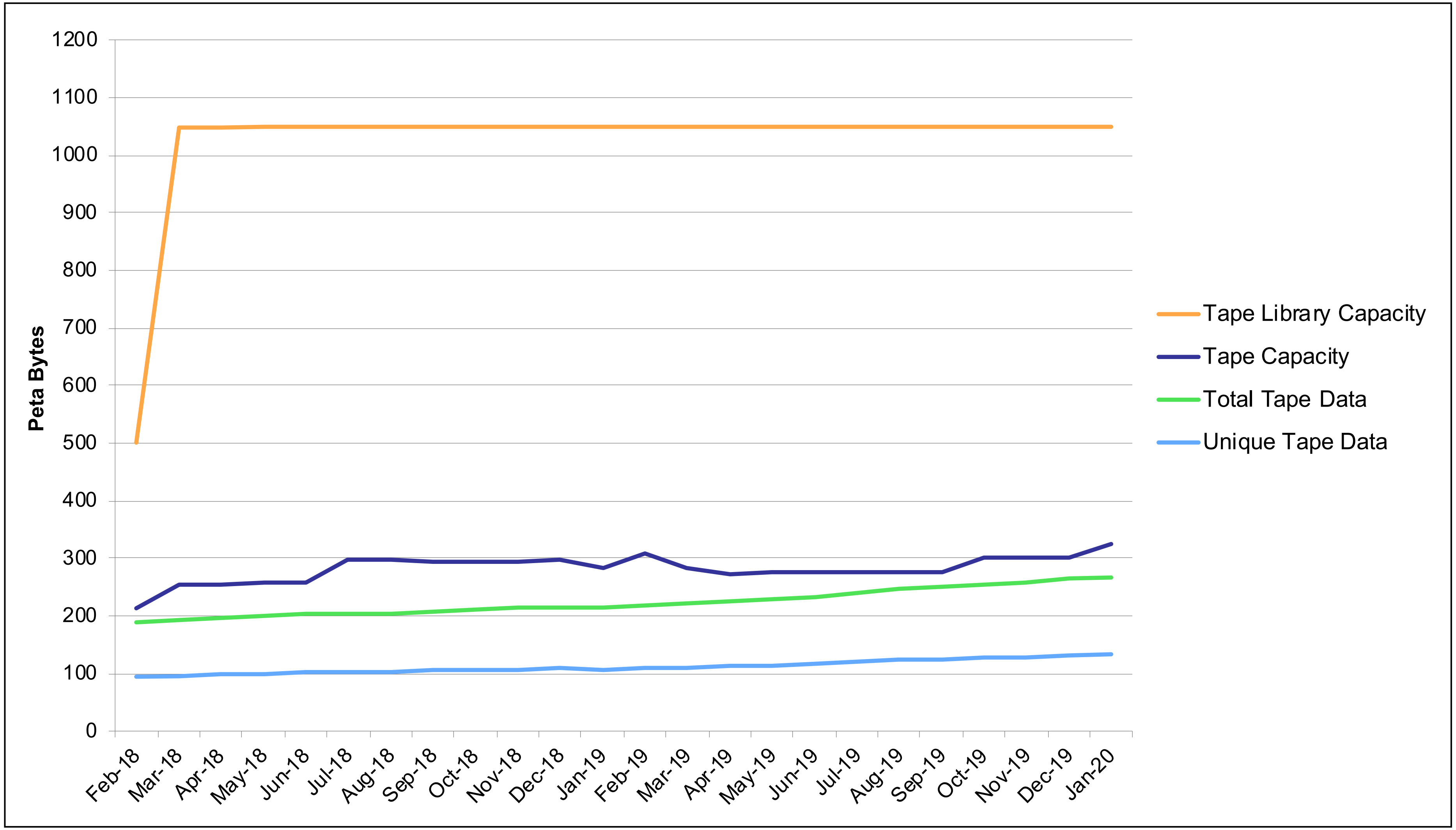
③ 2 Skylake E cells (8 D Rack Equivalence) added to Electra; 1 rack is dedicated to SMD

④ Skylake Tesla GPU V100 Nodes installed

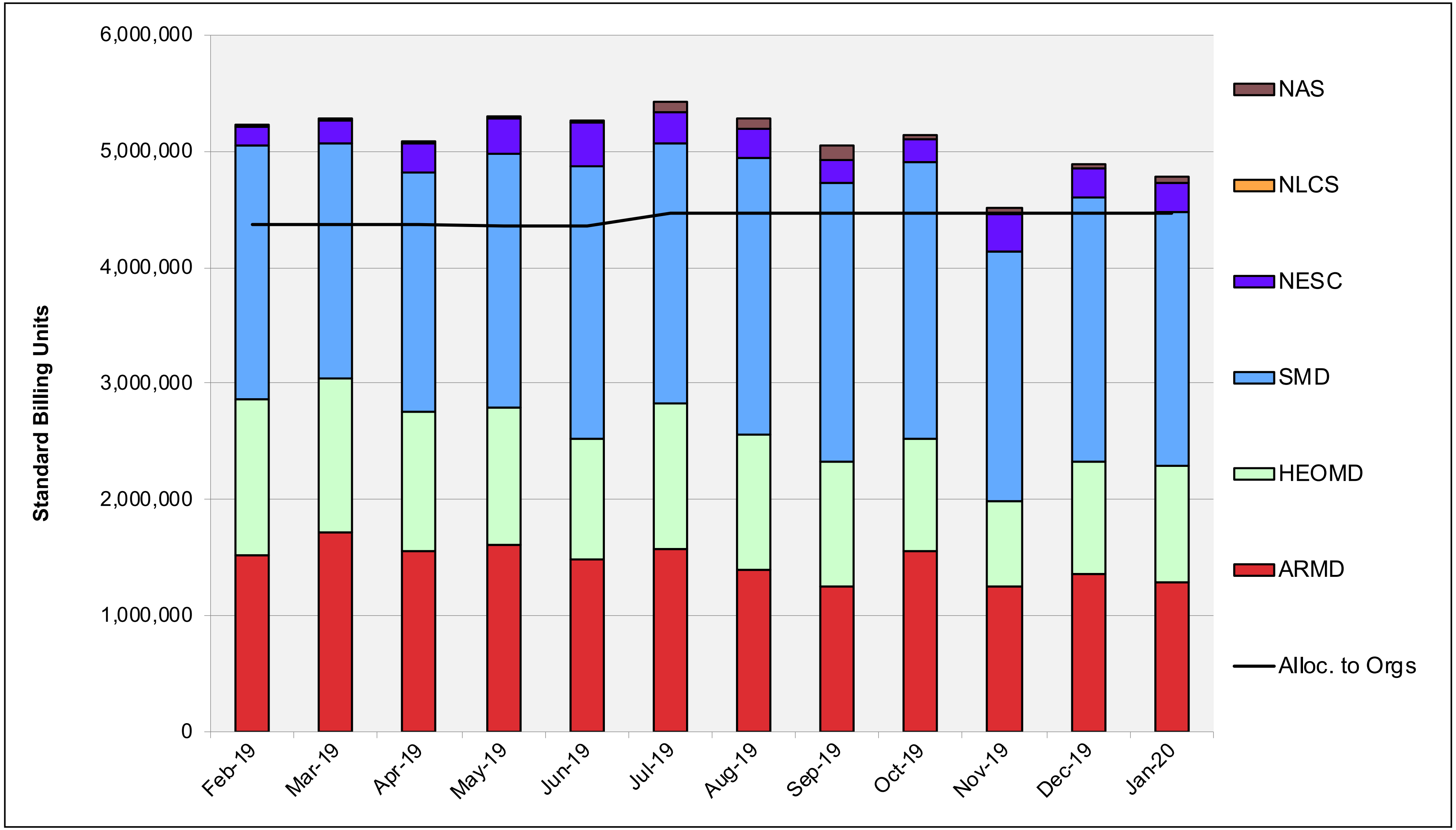
Tape Archive Status



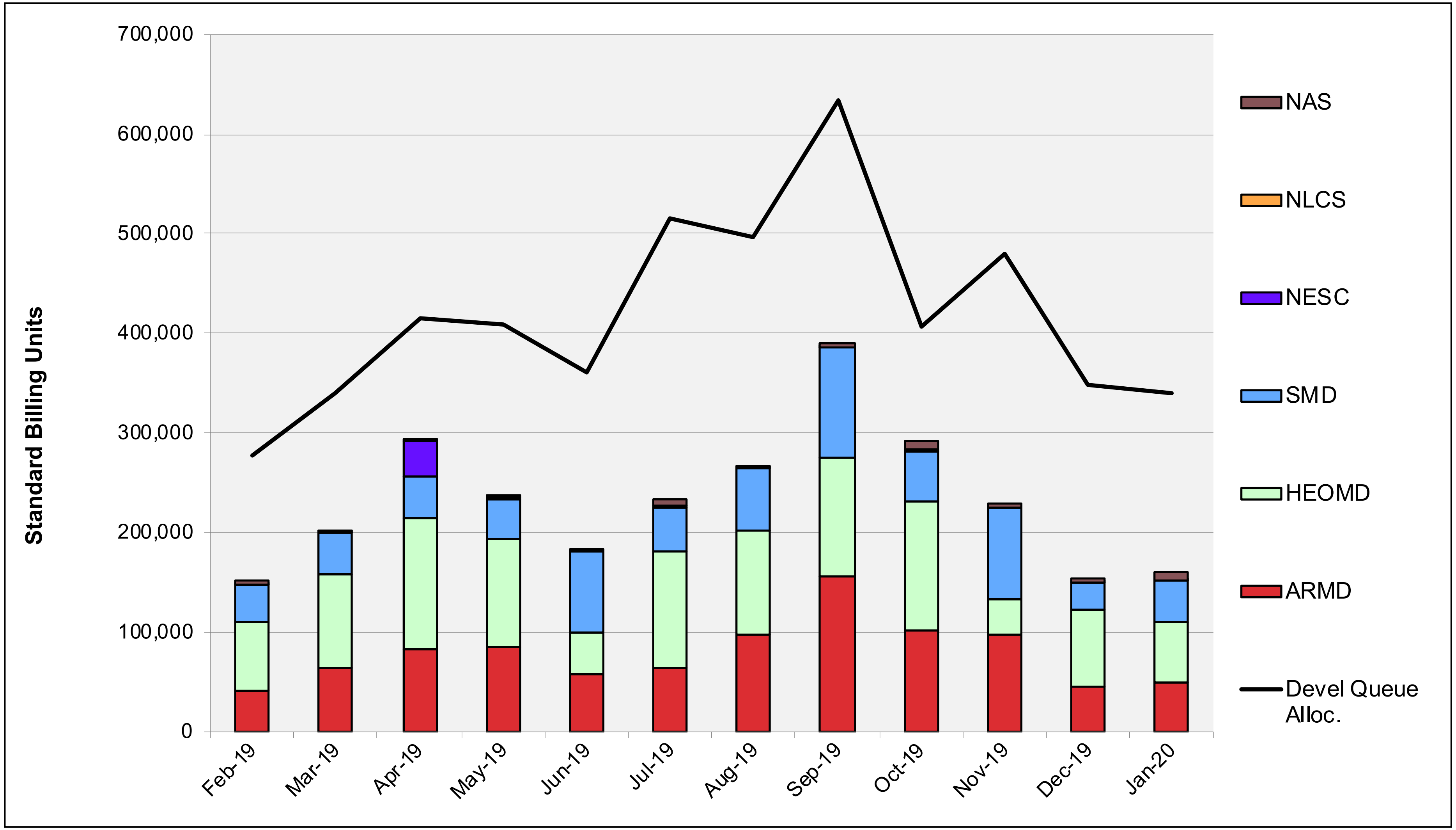
Tape Archive Status



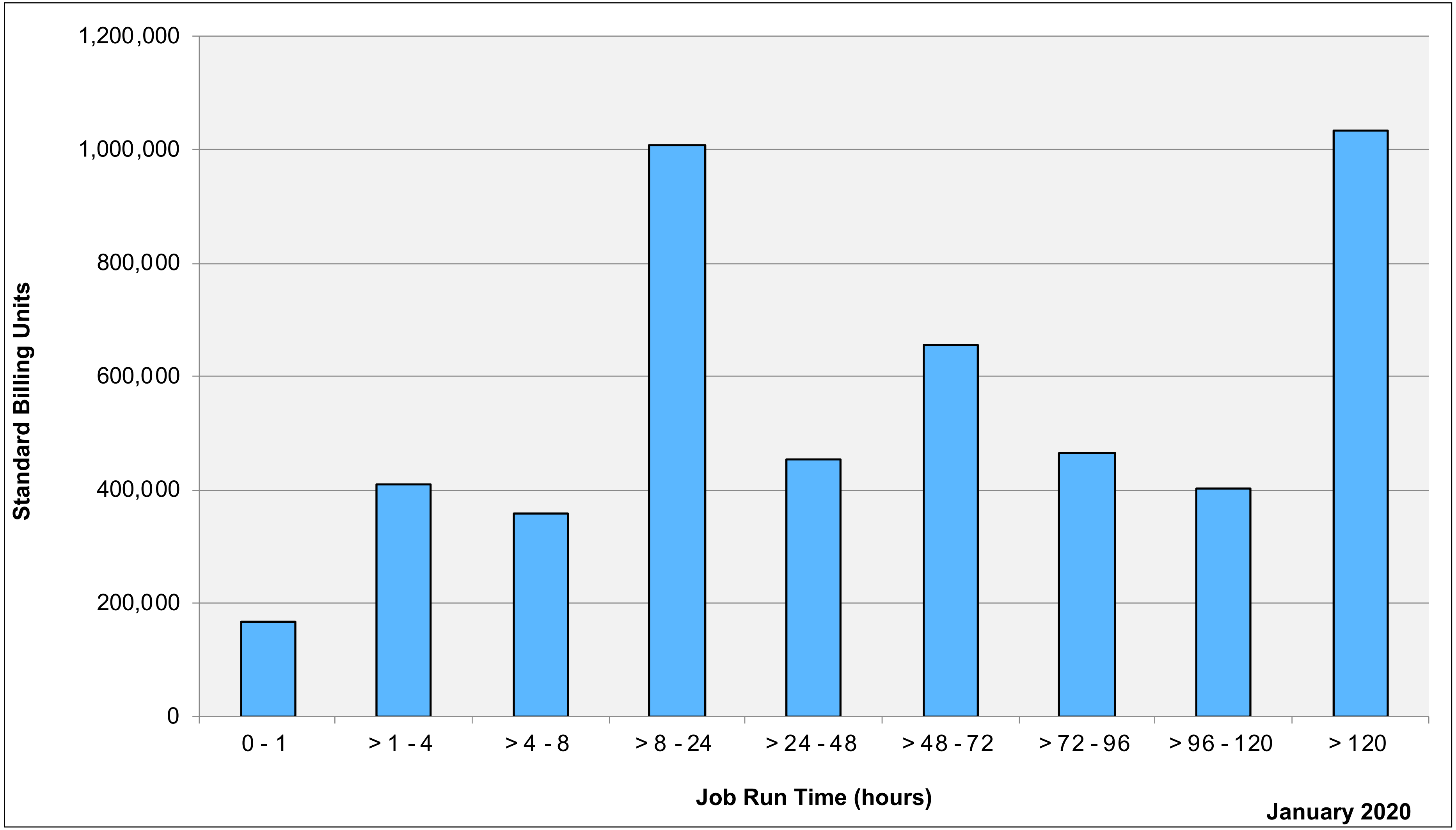
Pleiades: SBUs Reported, Normalized to 30-Day Month



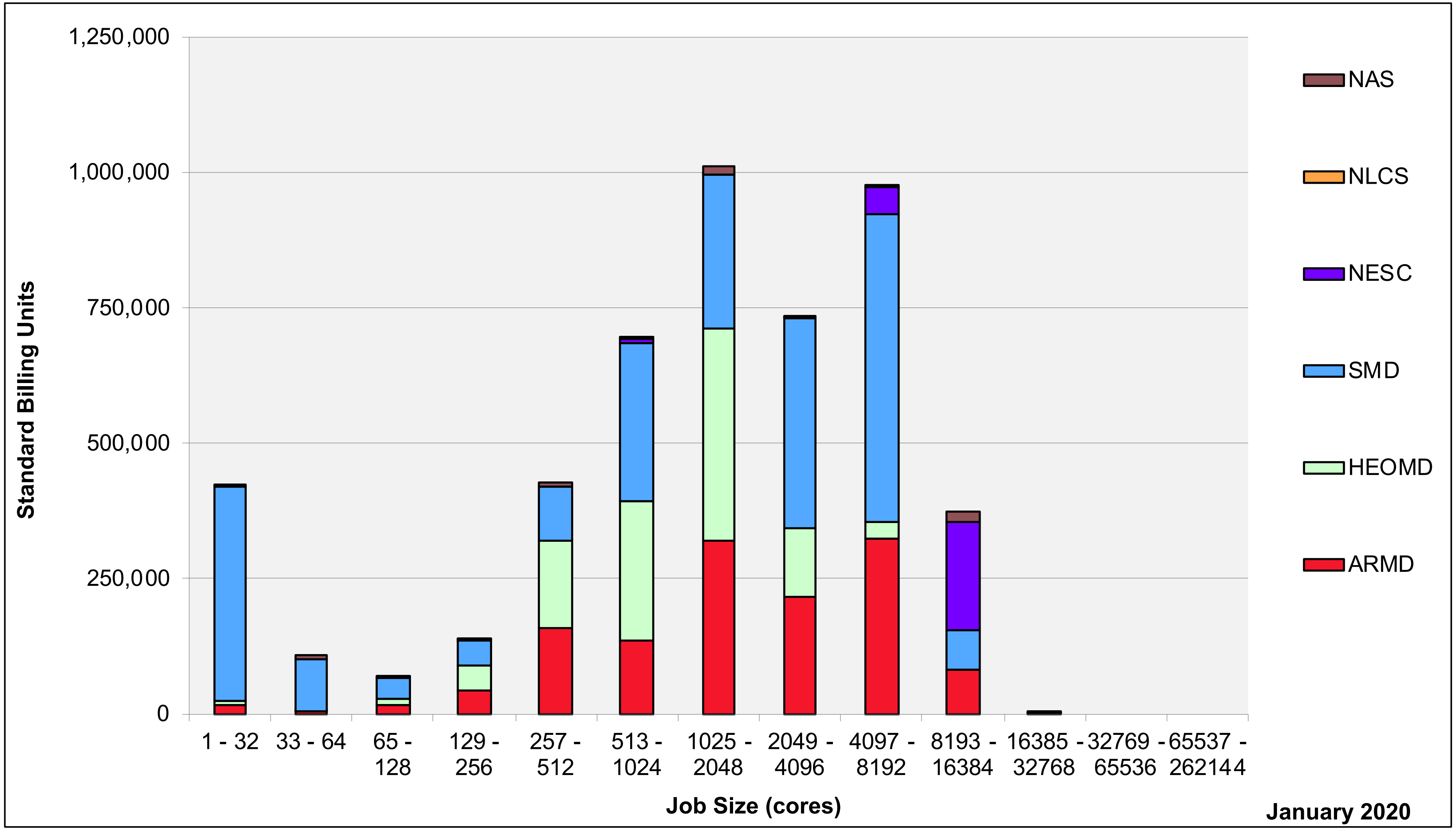
Pleiades: Devel Queue Utilization



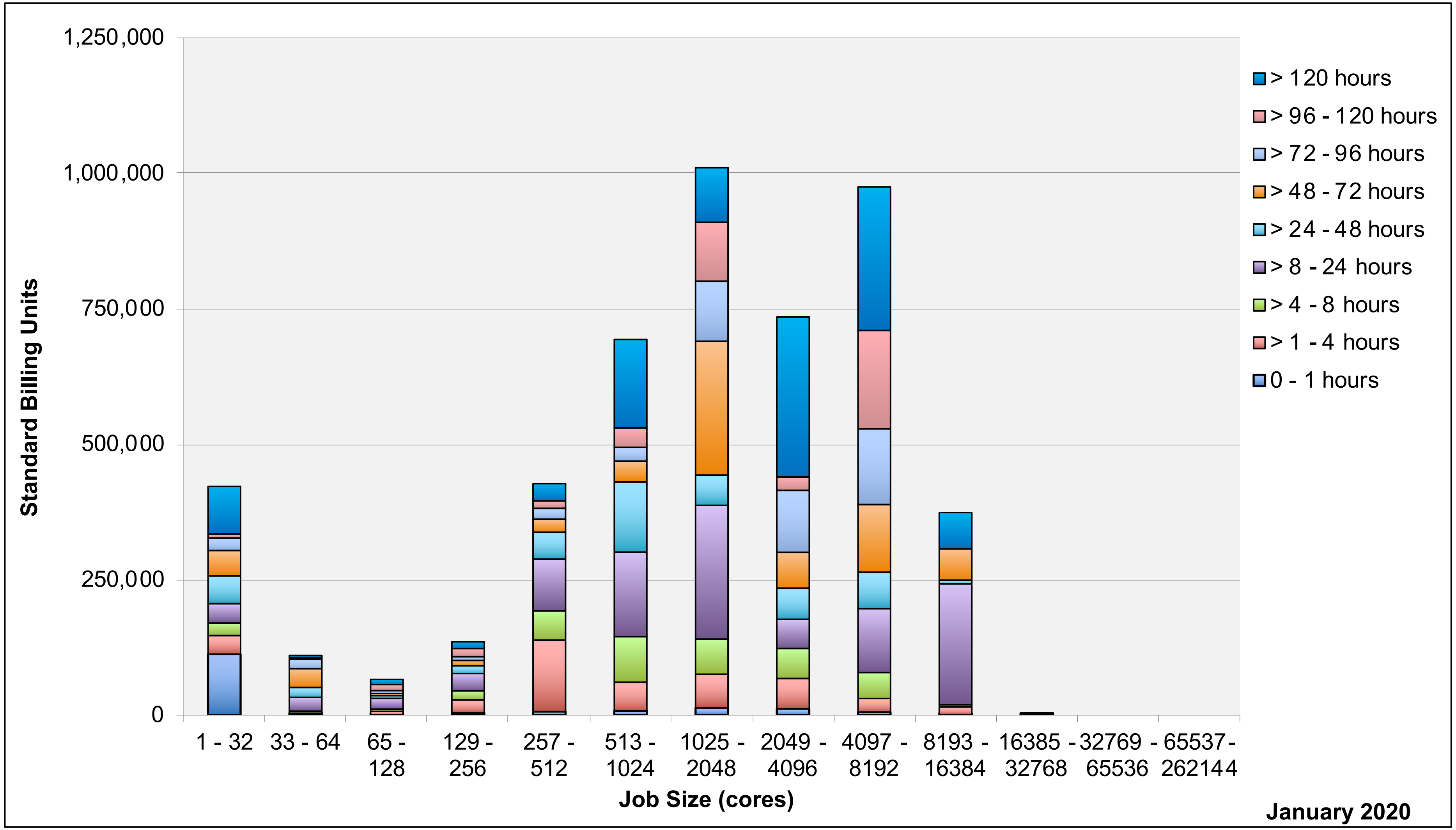
Pleiades: Monthly Utilization by Job Length



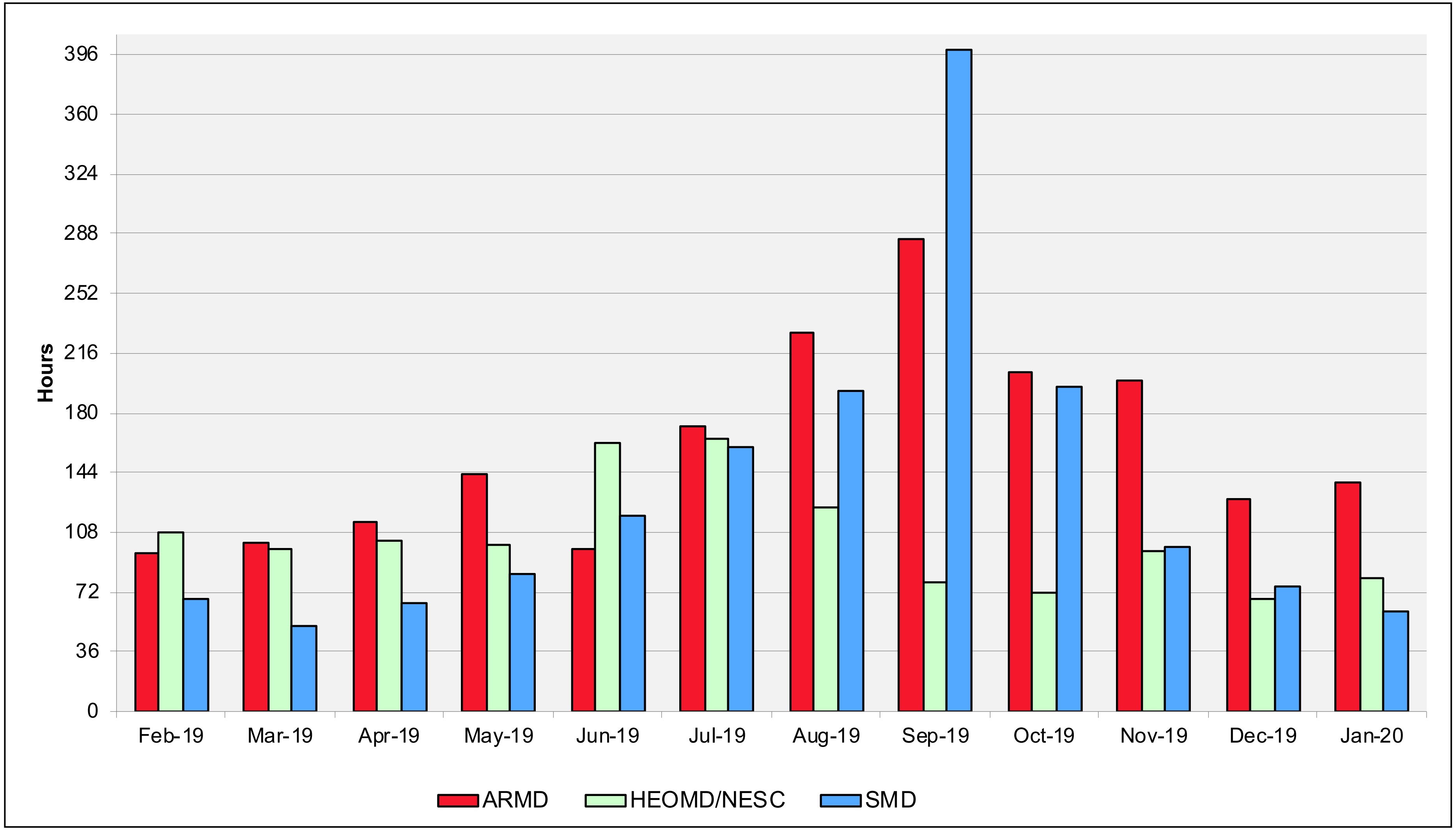
Pleiades: Monthly Utilization by Job Length



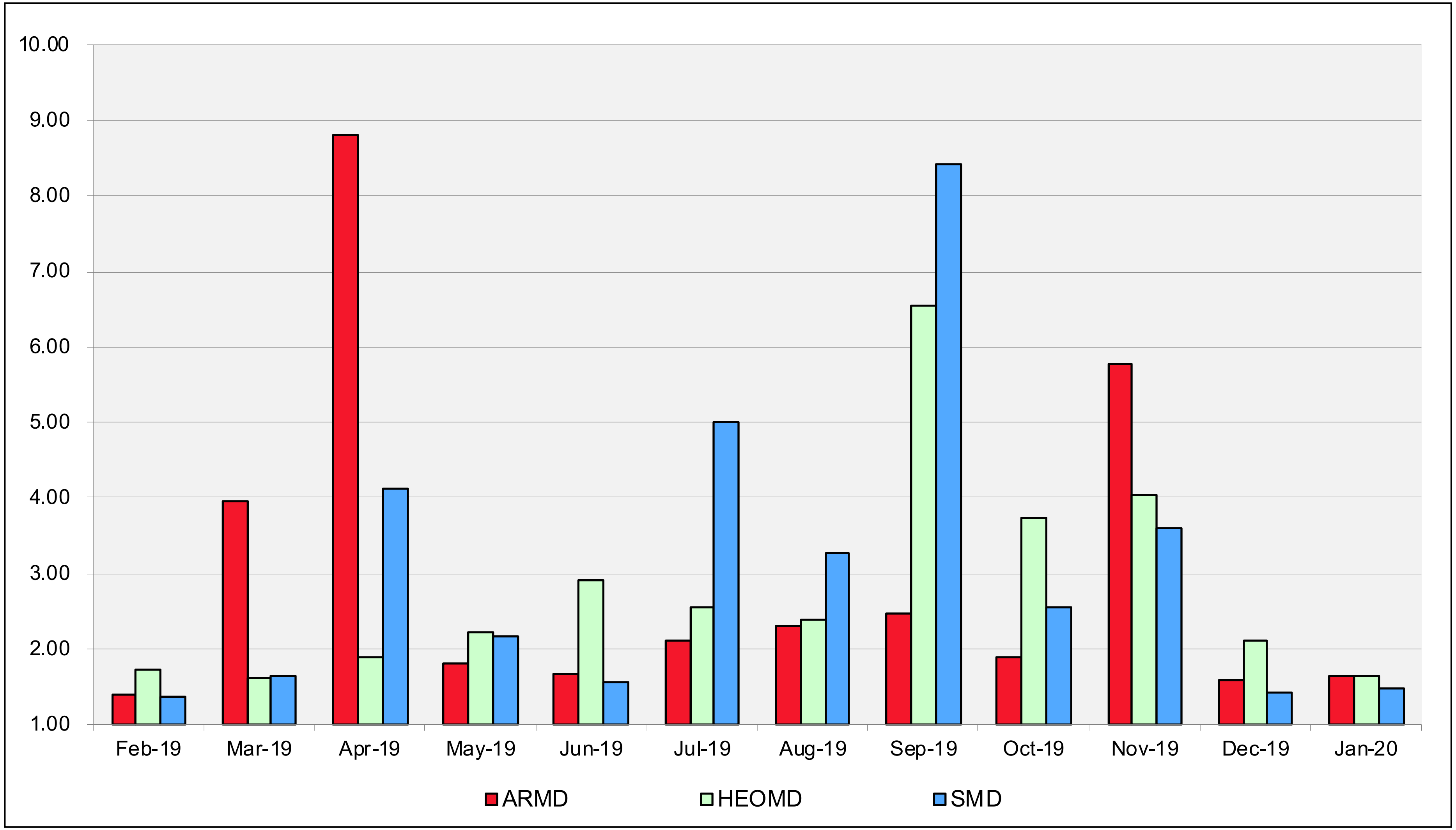
Pleiades: Monthly Utilization by Size and Length



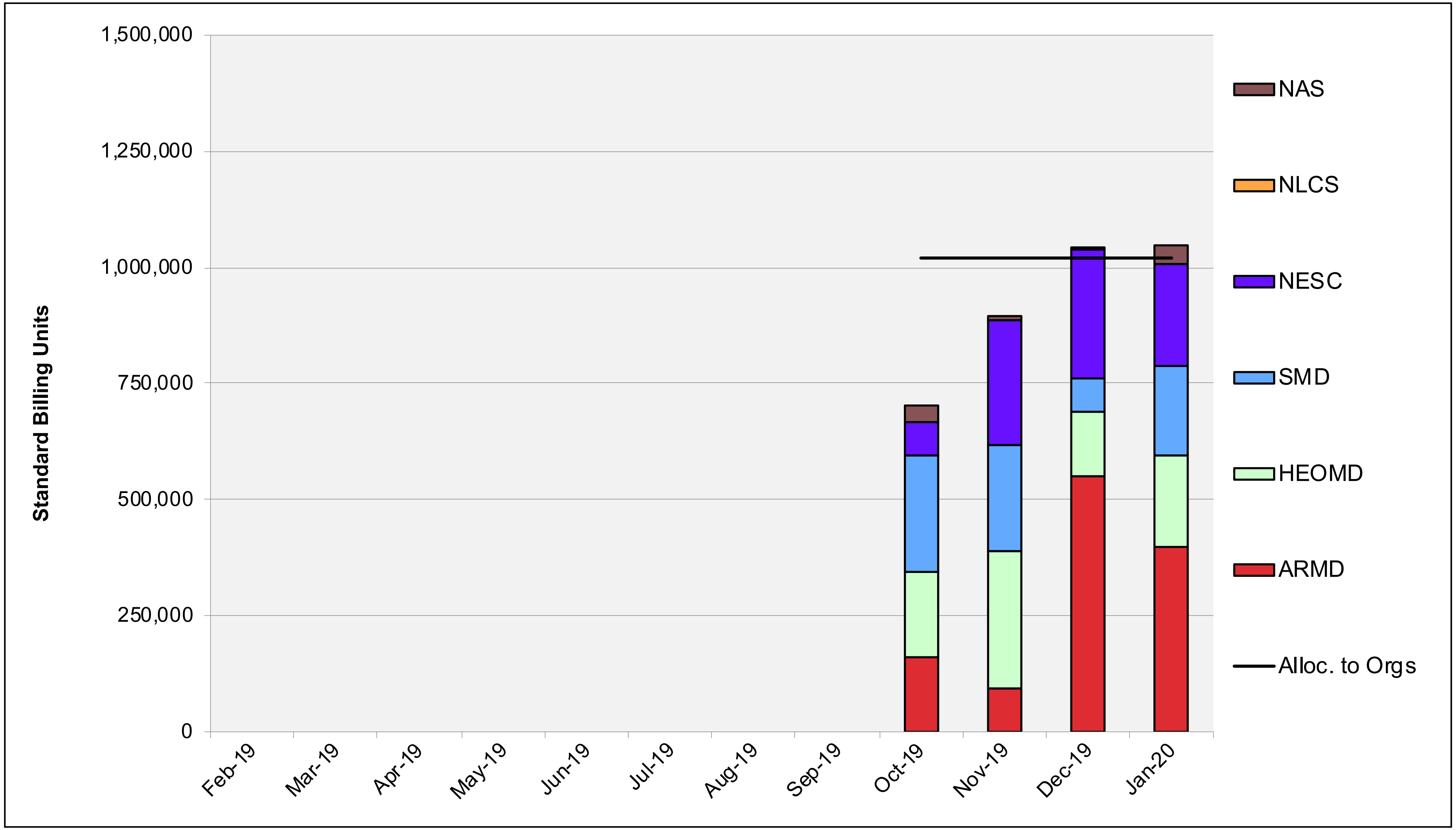
Pleiades: Average Time to Clear All Jobs



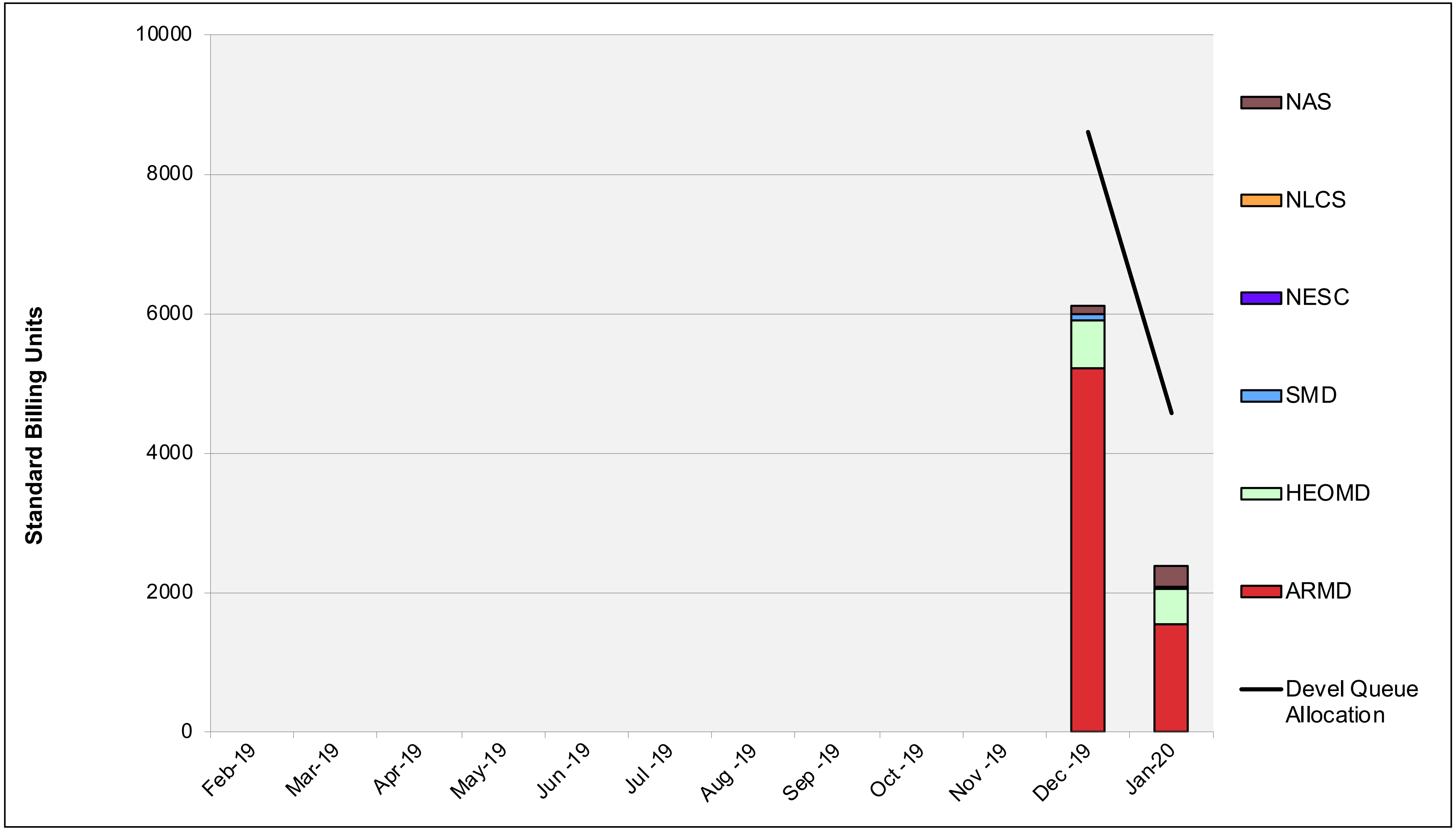
Pleiades: Average Expansion Factor



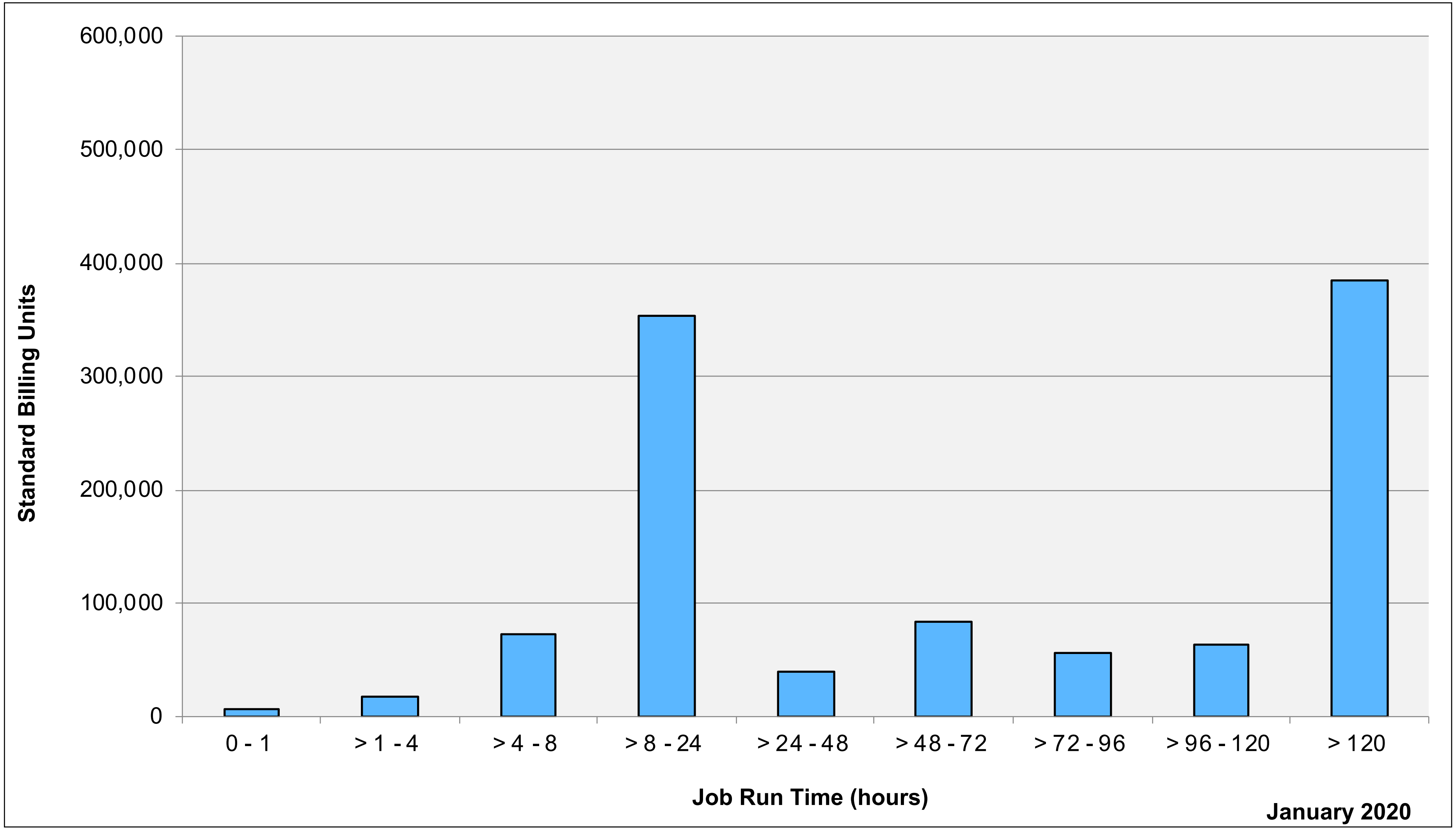
Aitken: SBUs Reported, Normalized to 30-Day Month



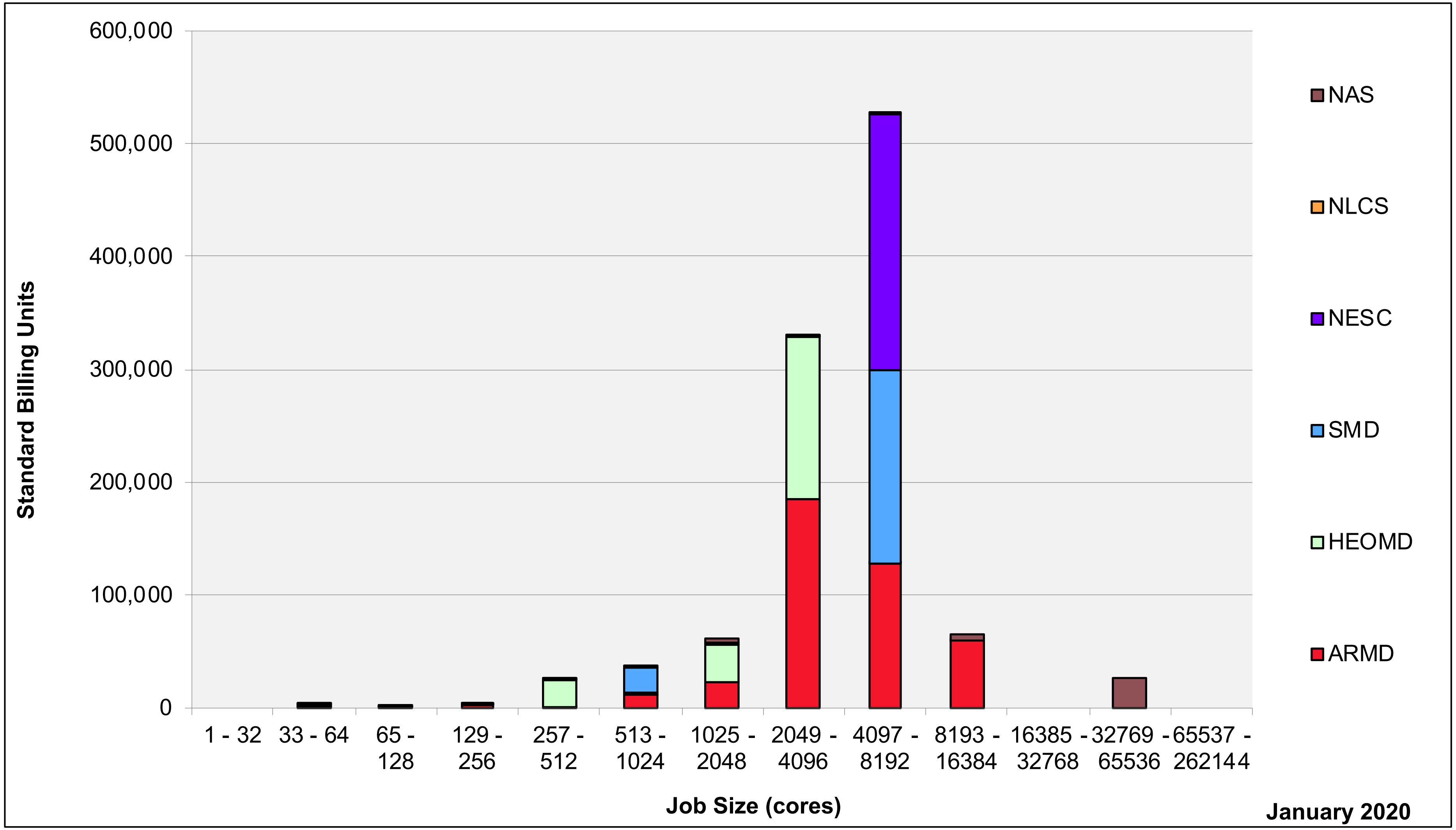
Aitken: Devel Queue Utilization



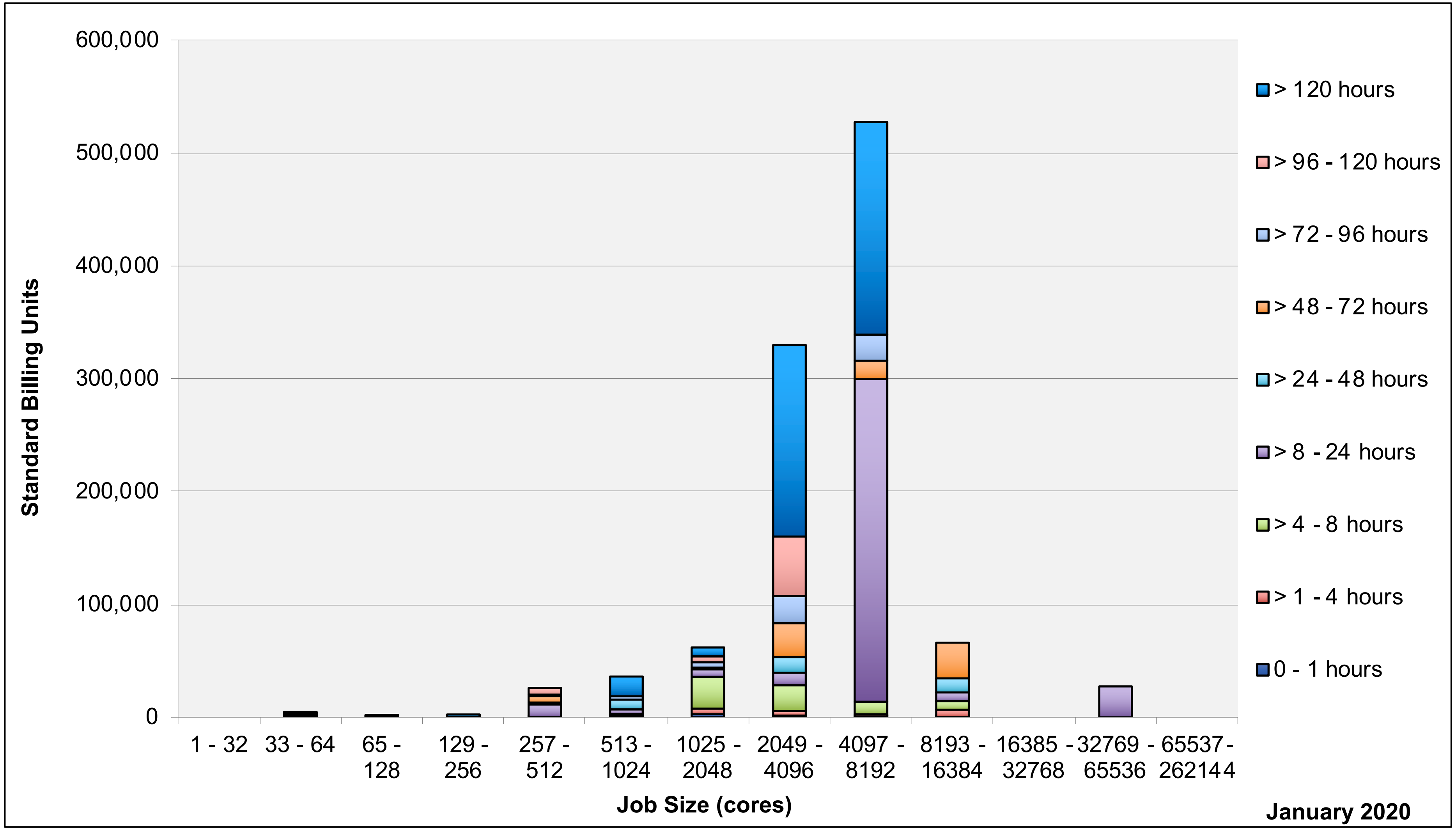
Aitken: Monthly Utilization by Job Length



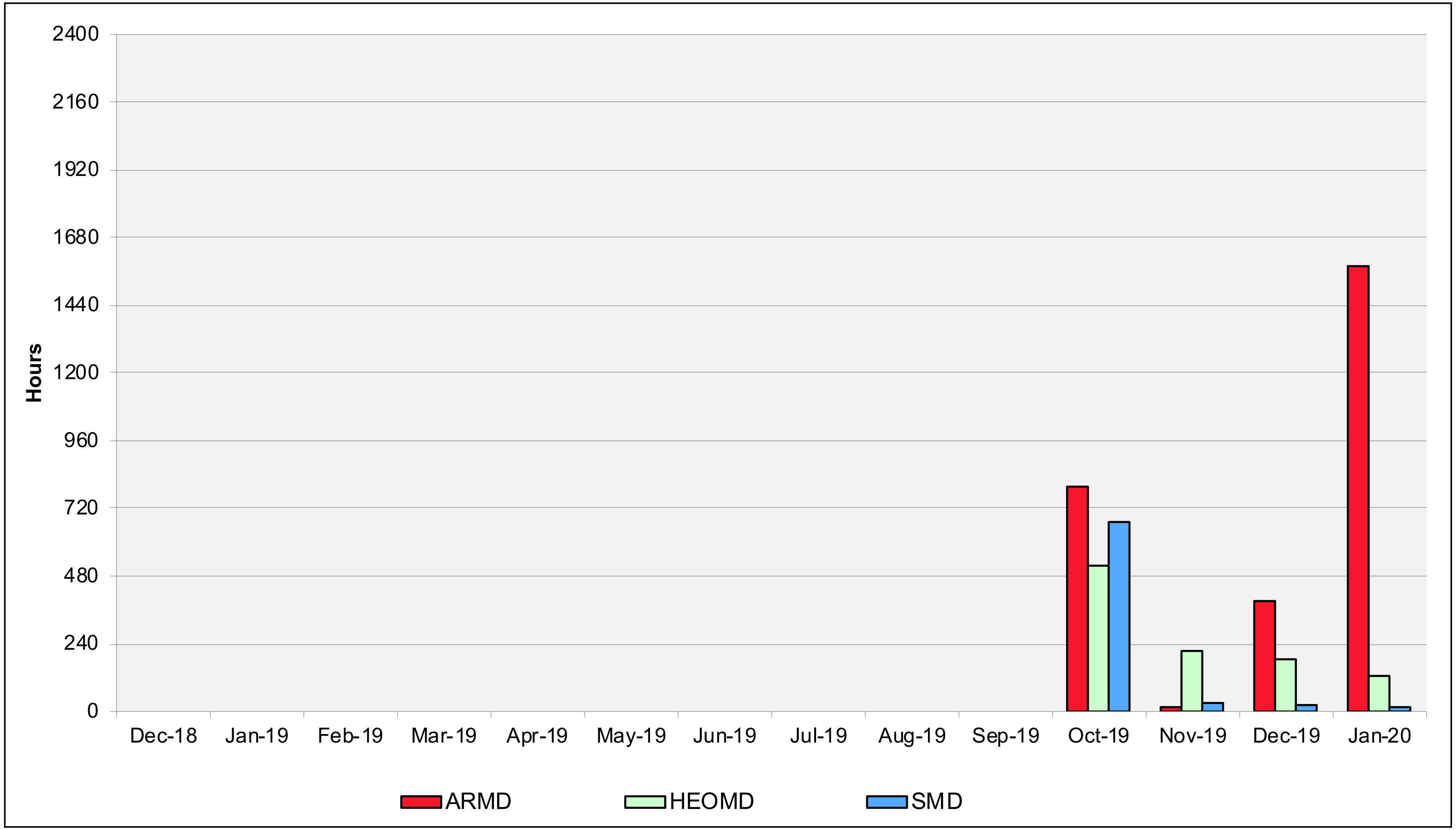
Aitken: Monthly Utilization by Job Length



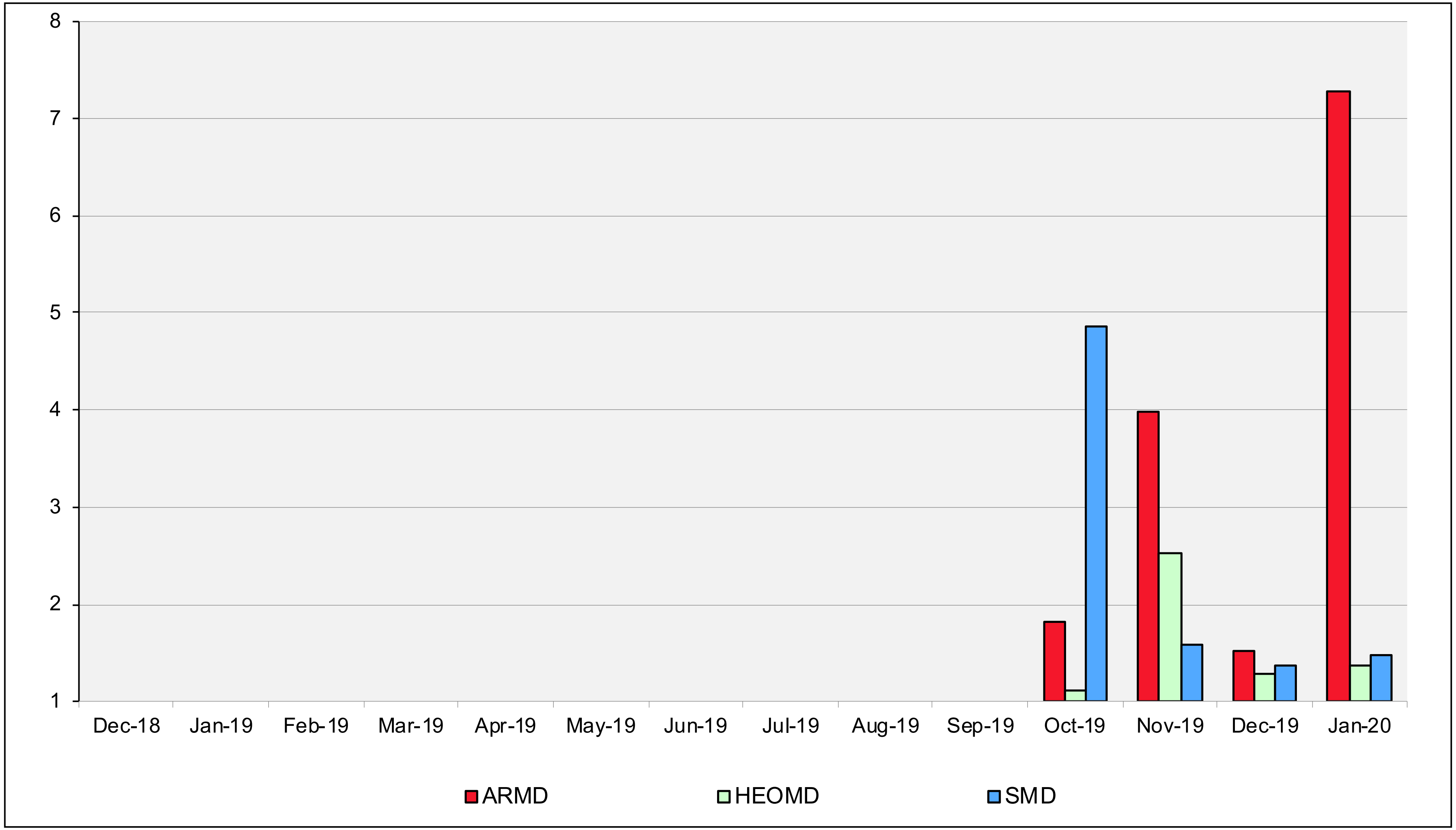
Aitken: Monthly Utilization by Size and Length



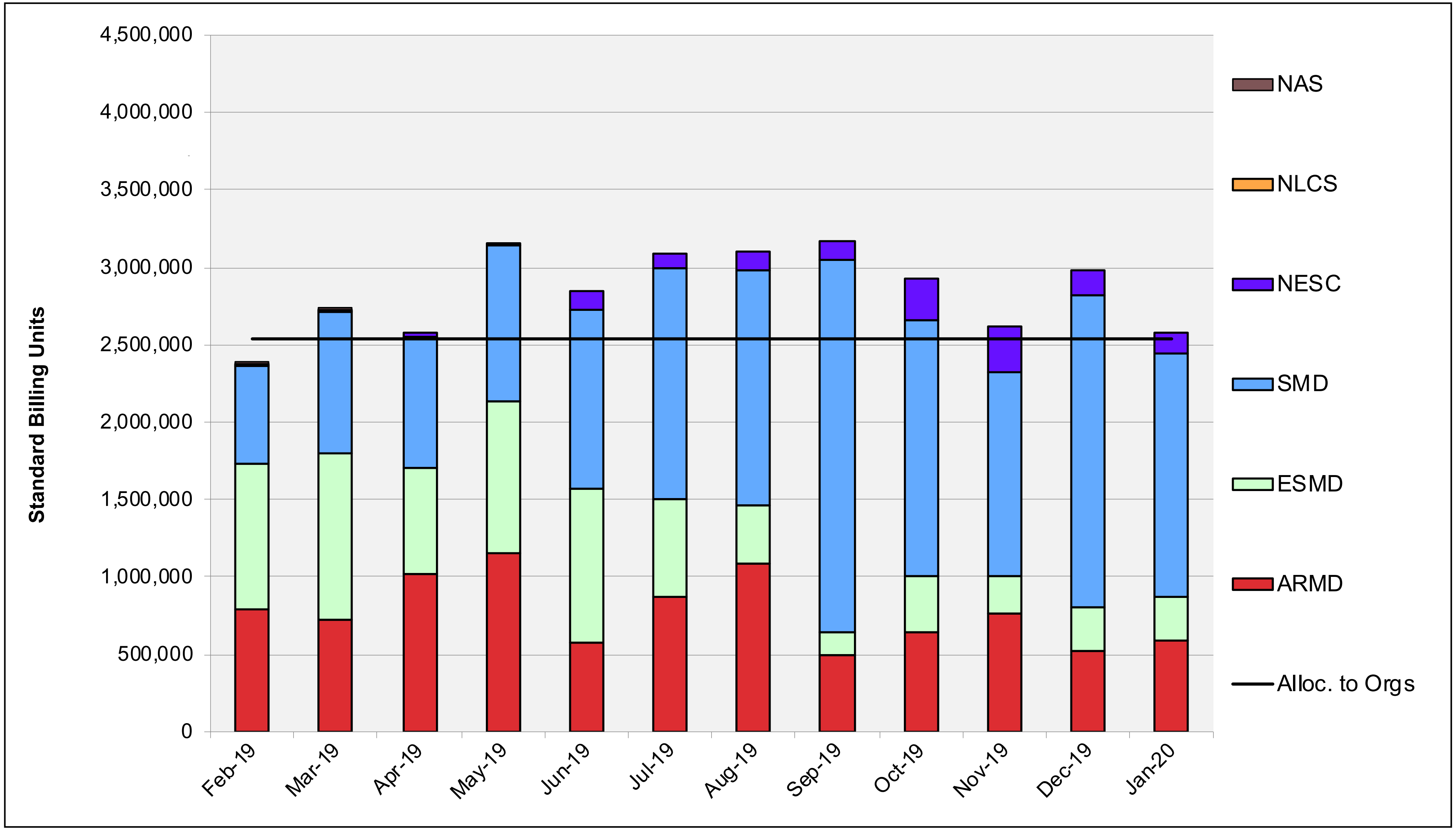
Aitken: Average Time to Clear All Jobs



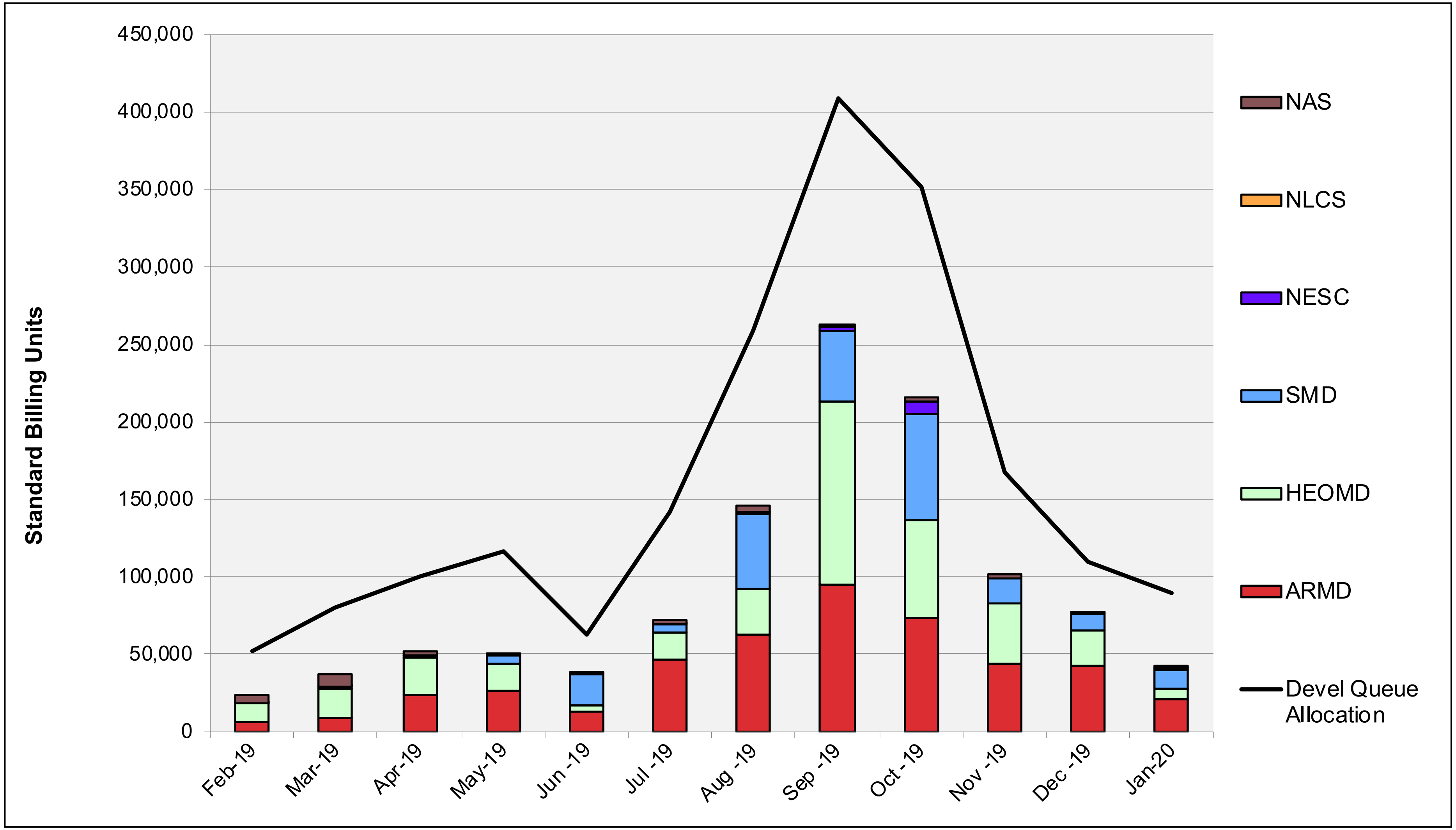
Aitken: Average Expansion Factor



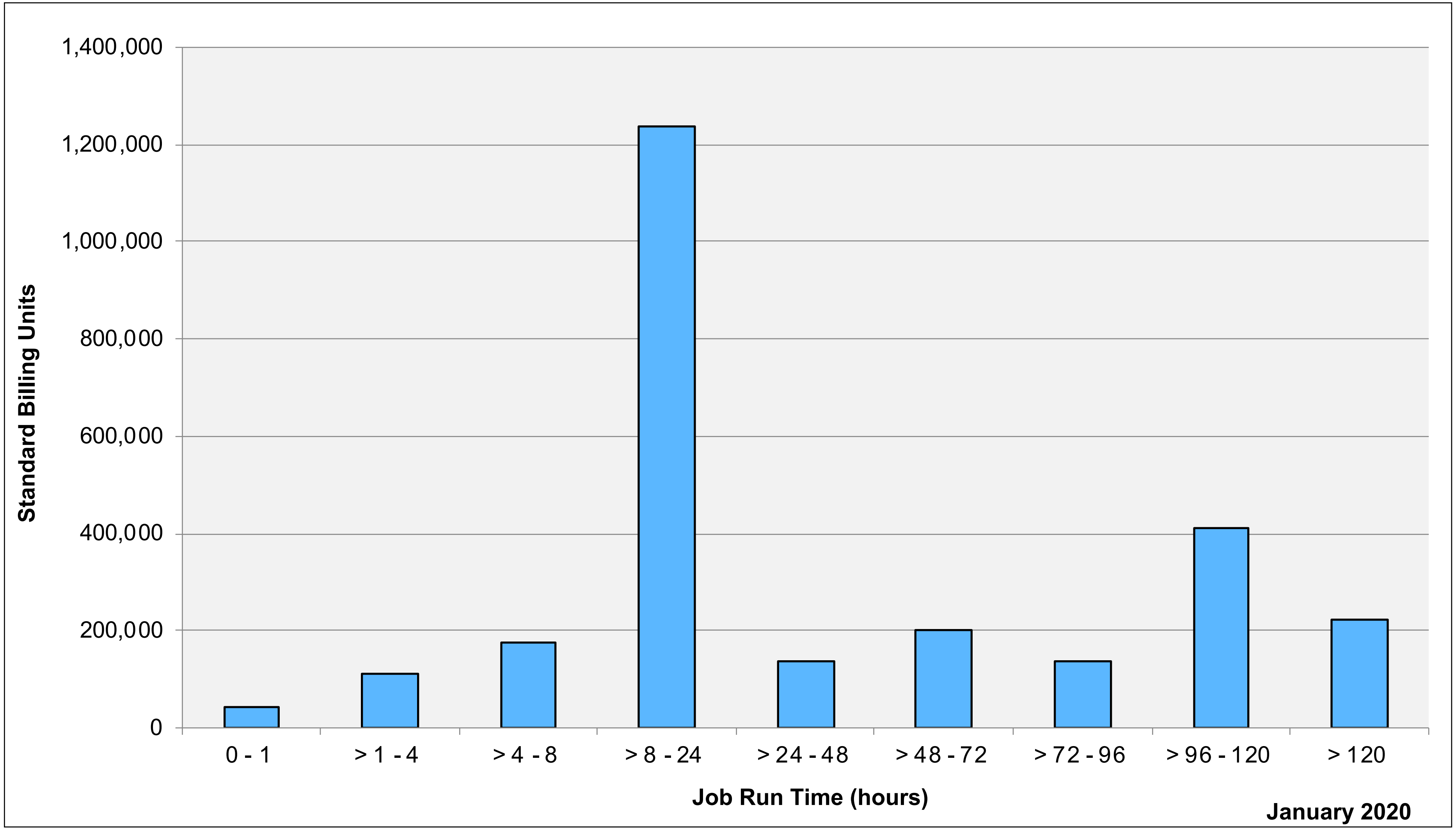
Electra: SBUs Reported, Normalized to 30-Day Month



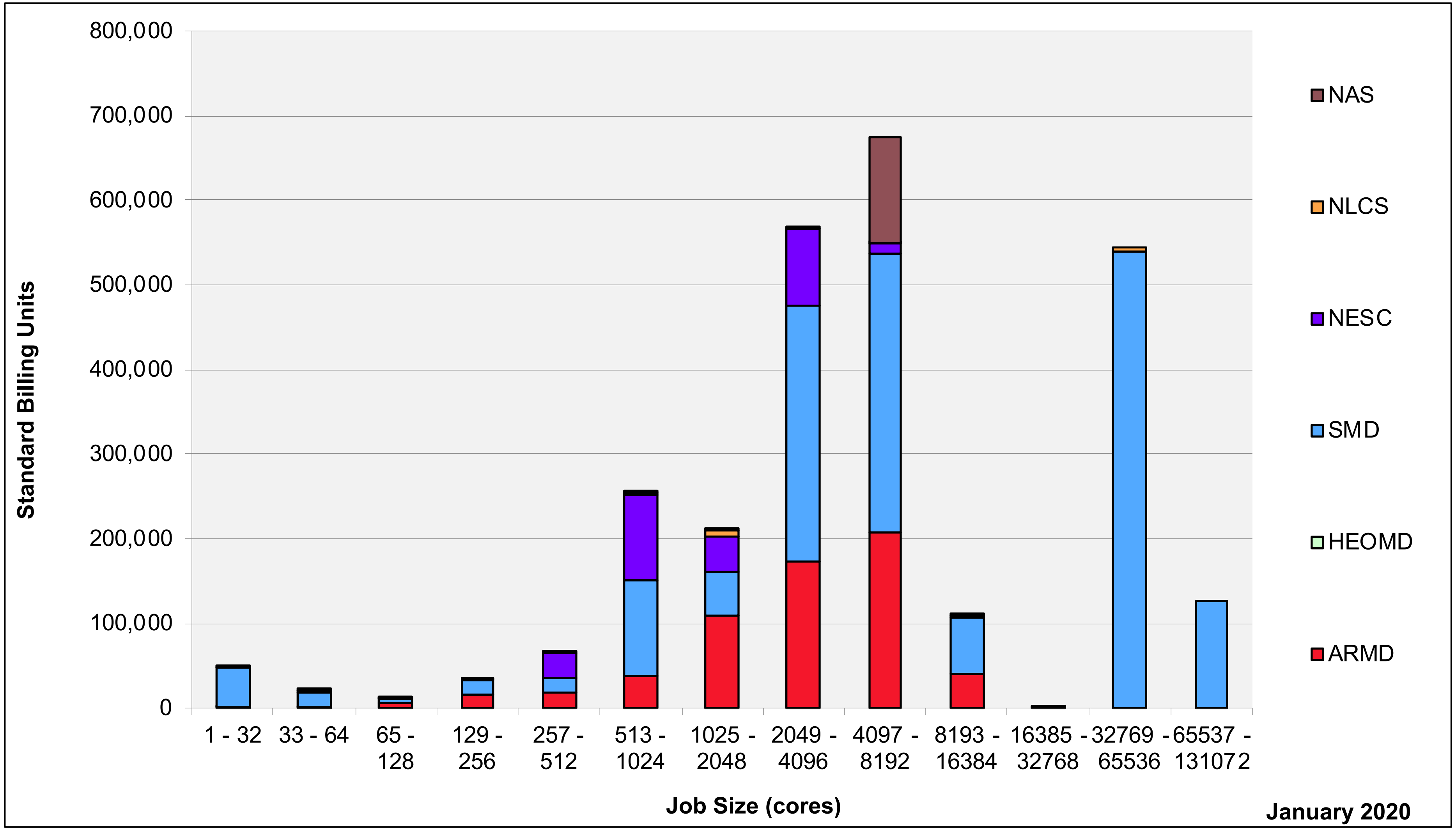
Electra: Devel Queue Utilization



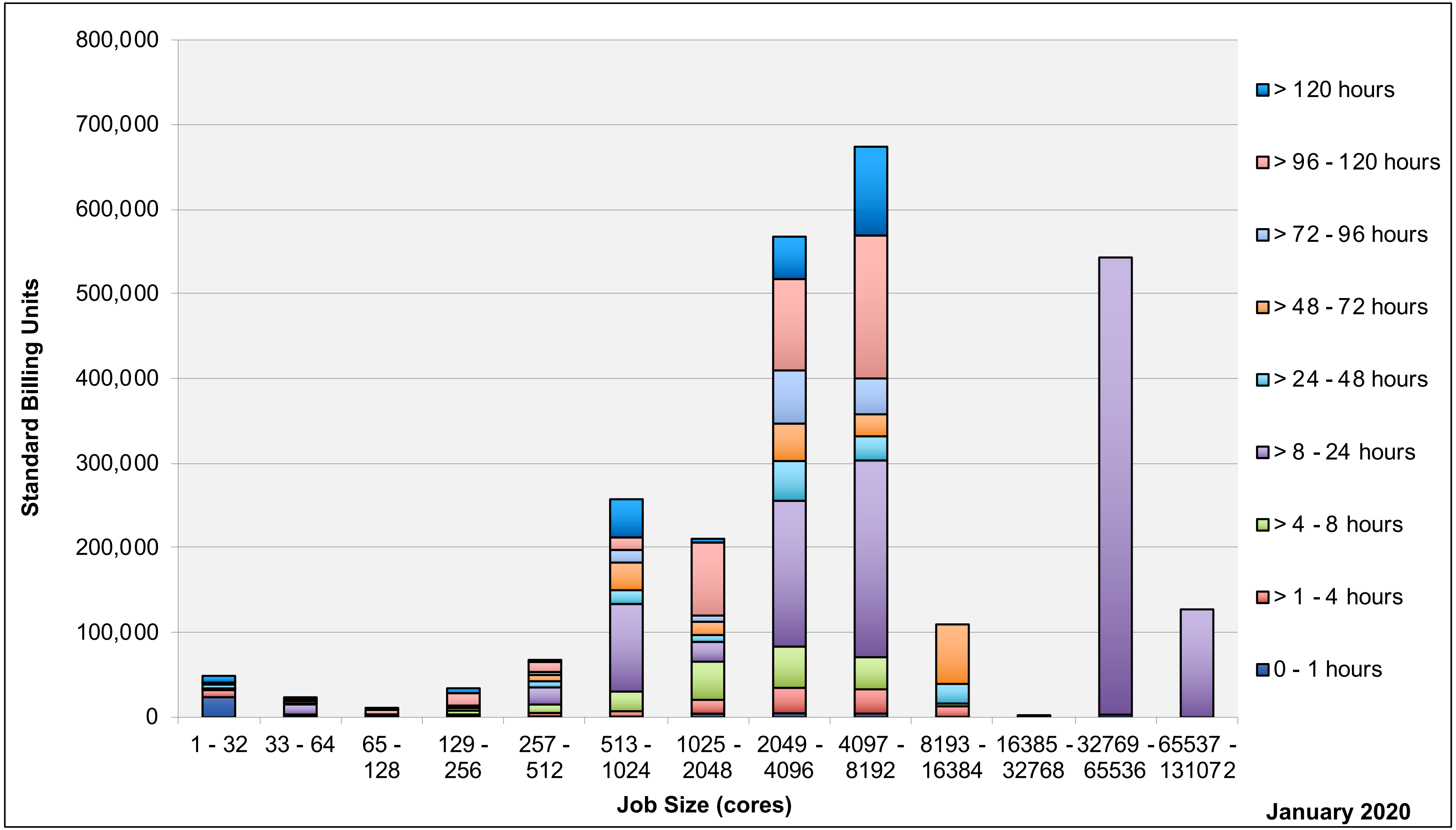
Electra: Monthly Utilization by Job Length



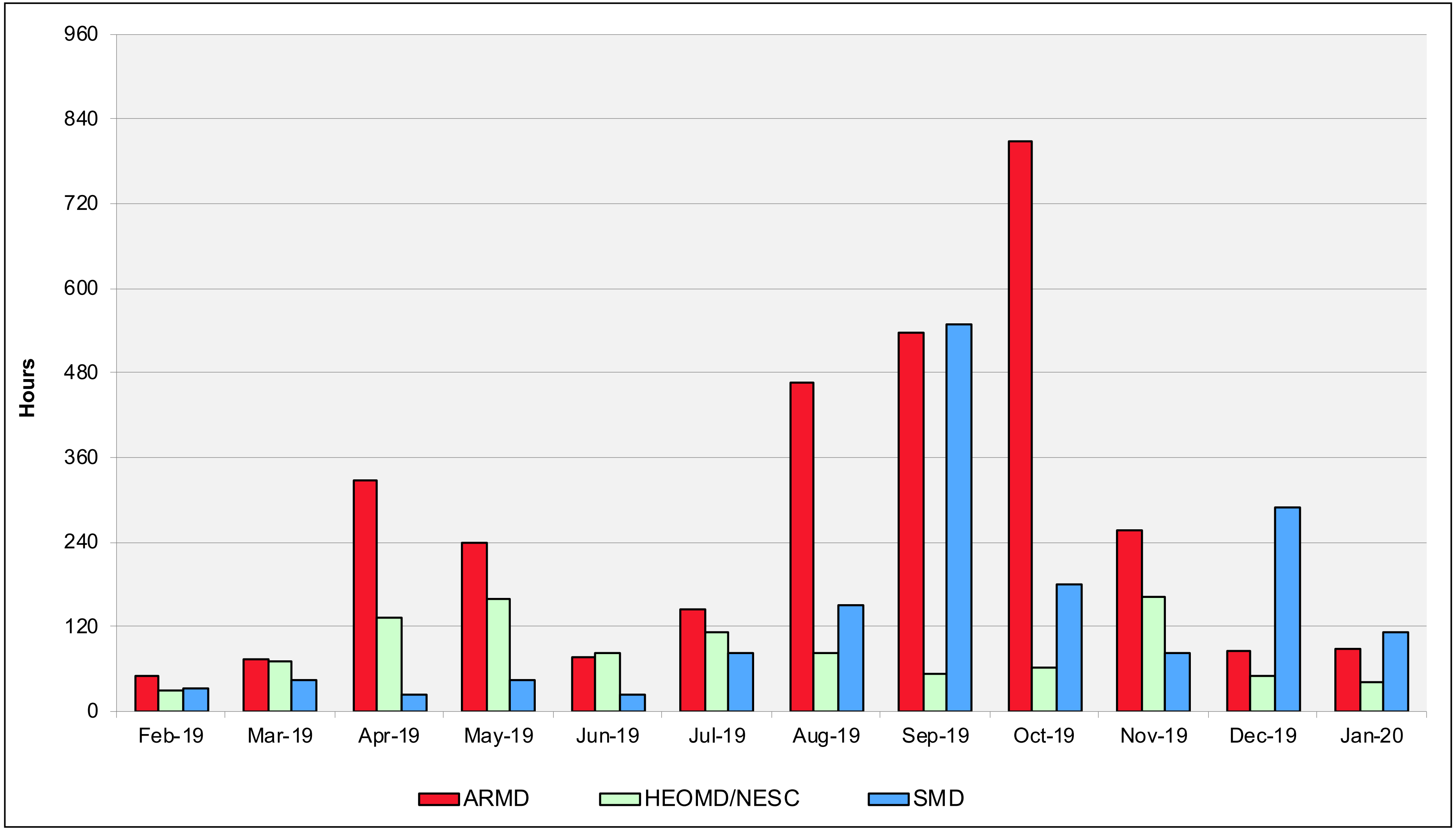
Electra: Monthly Utilization by Job Length



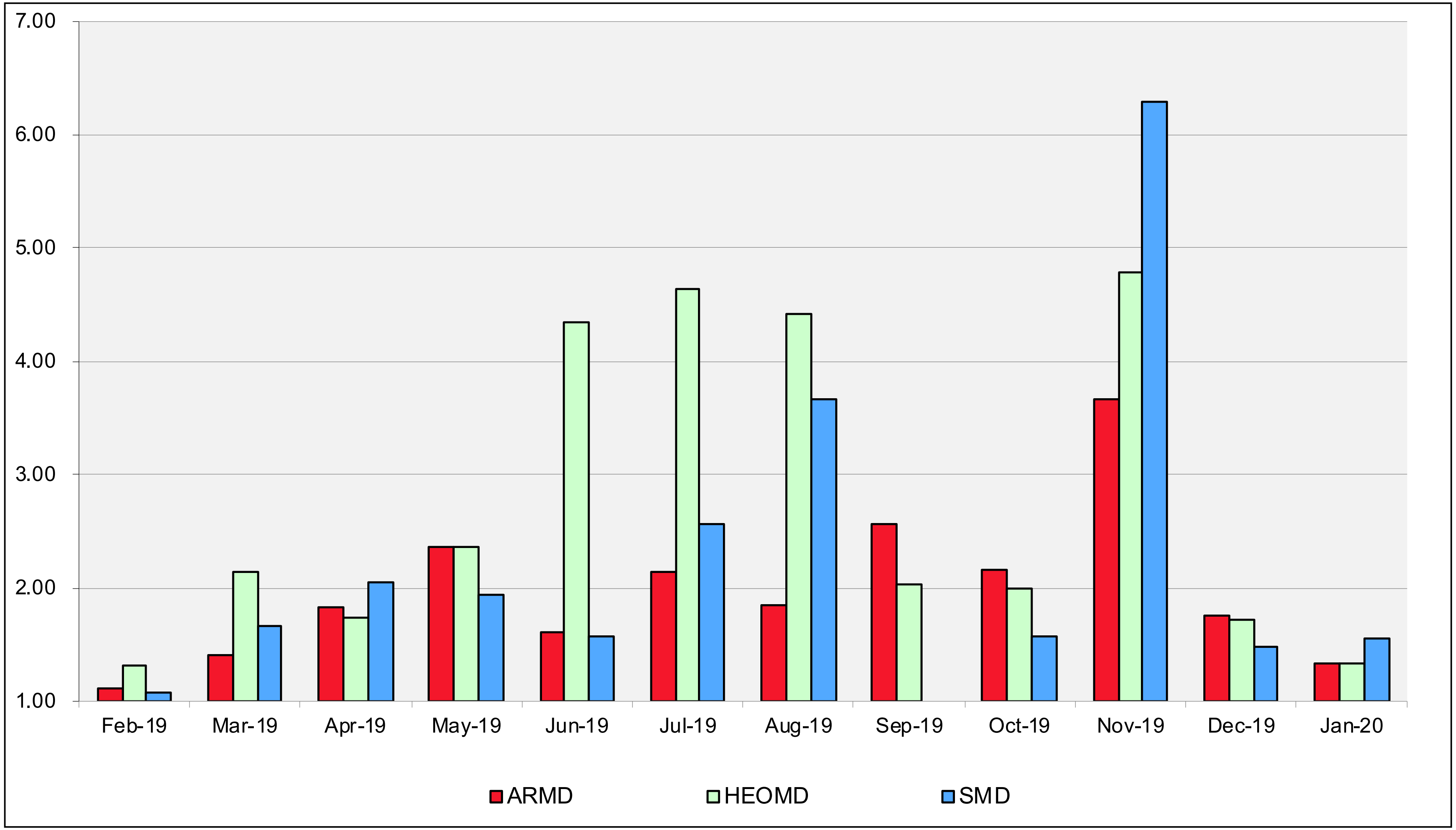
Electra: Monthly Utilization by Size and Length



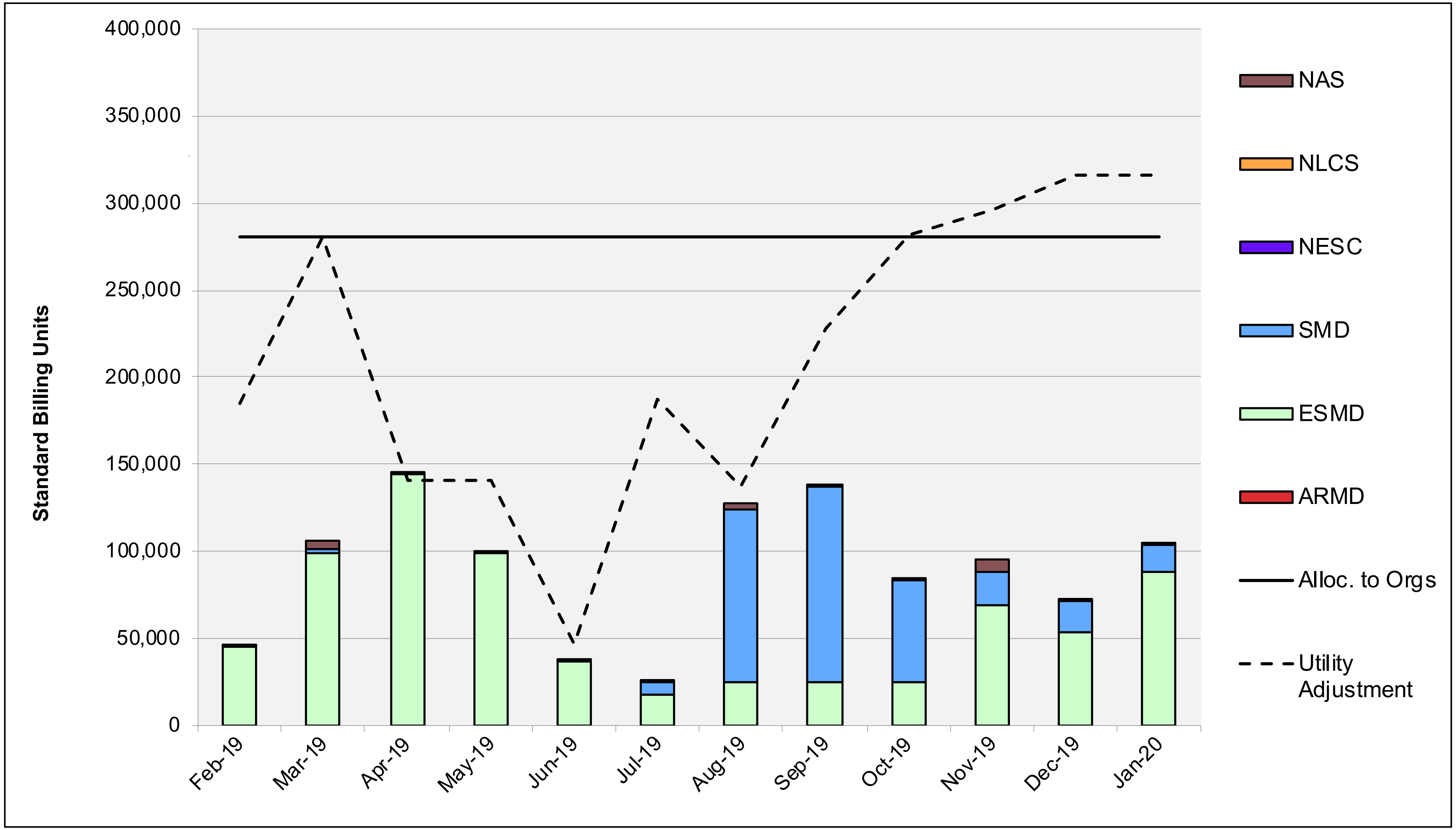
Electra: Average Time to Clear All Jobs



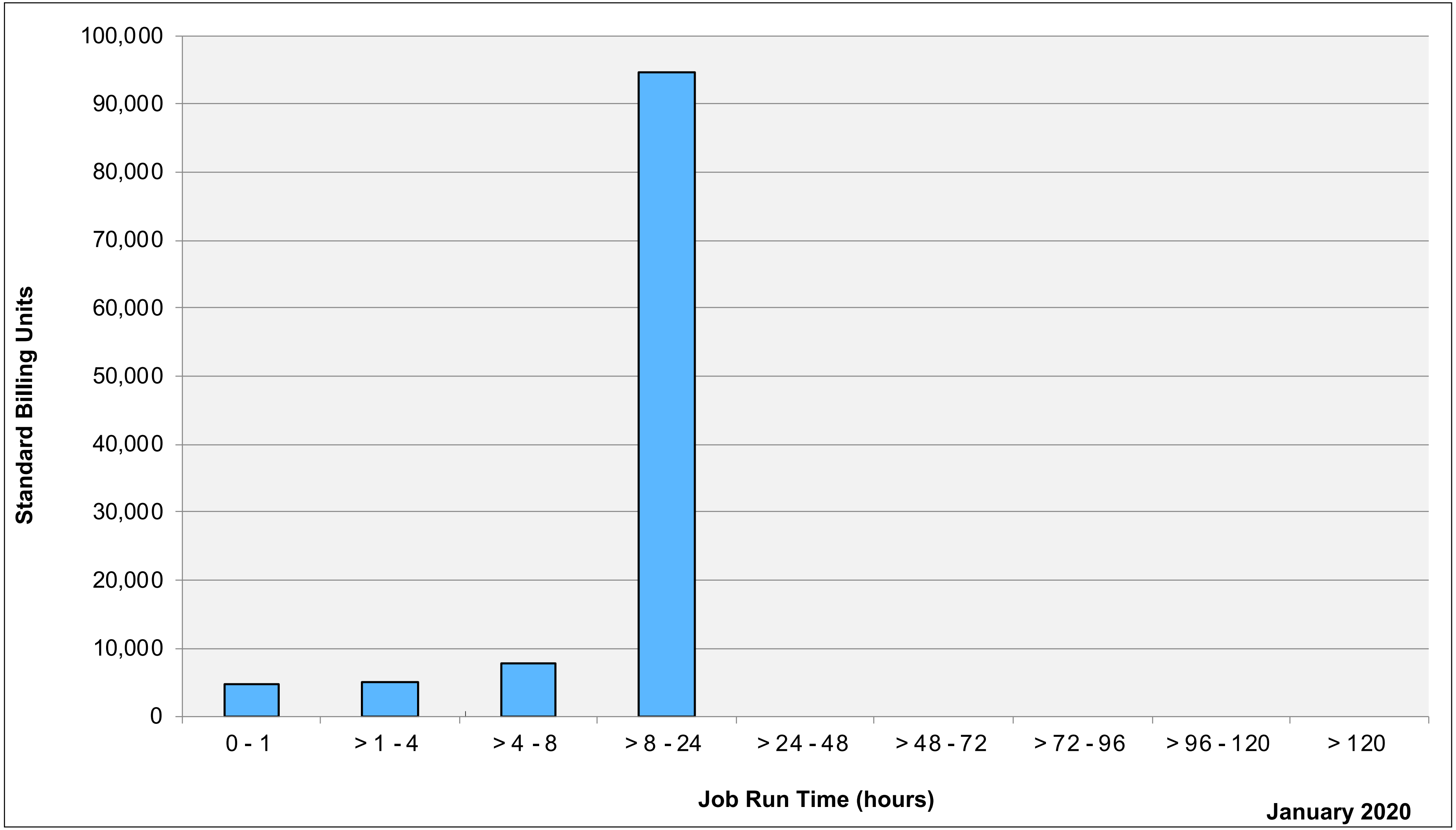
Electra: Average Expansion Factor



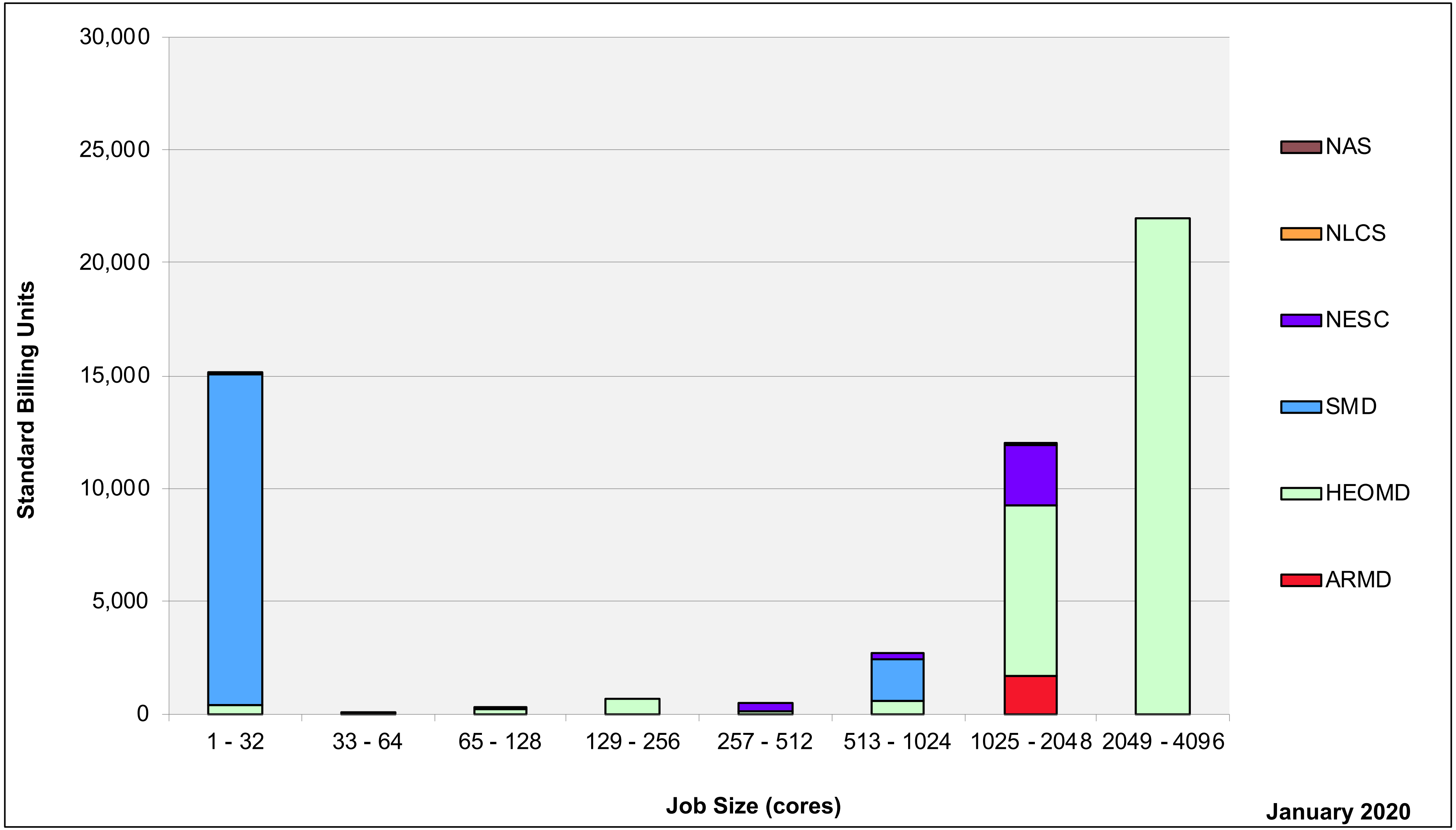
Merope: SBUs Reported, Normalized to 30-Day Month



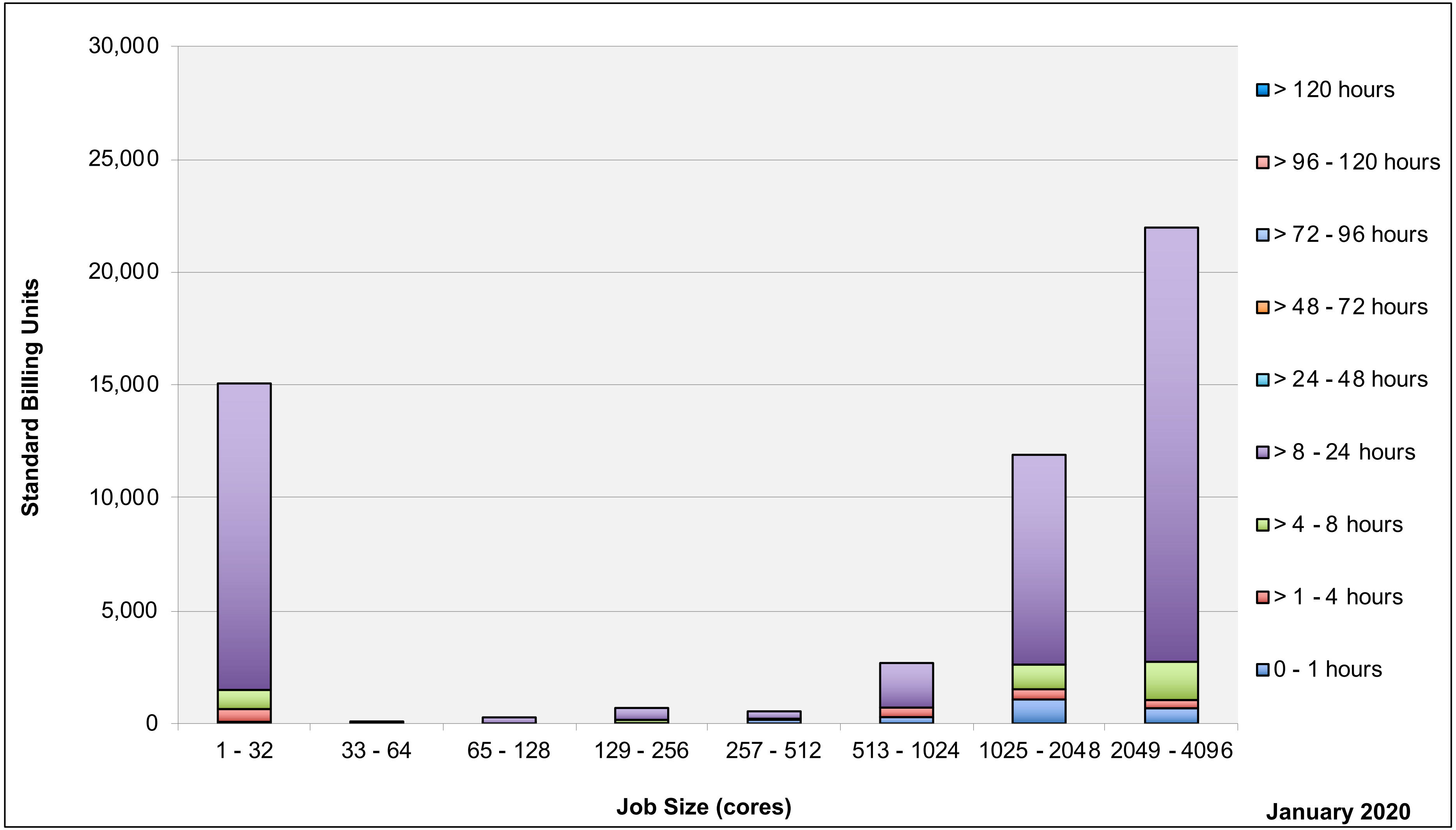
Merope: Monthly Utilization by Job Length



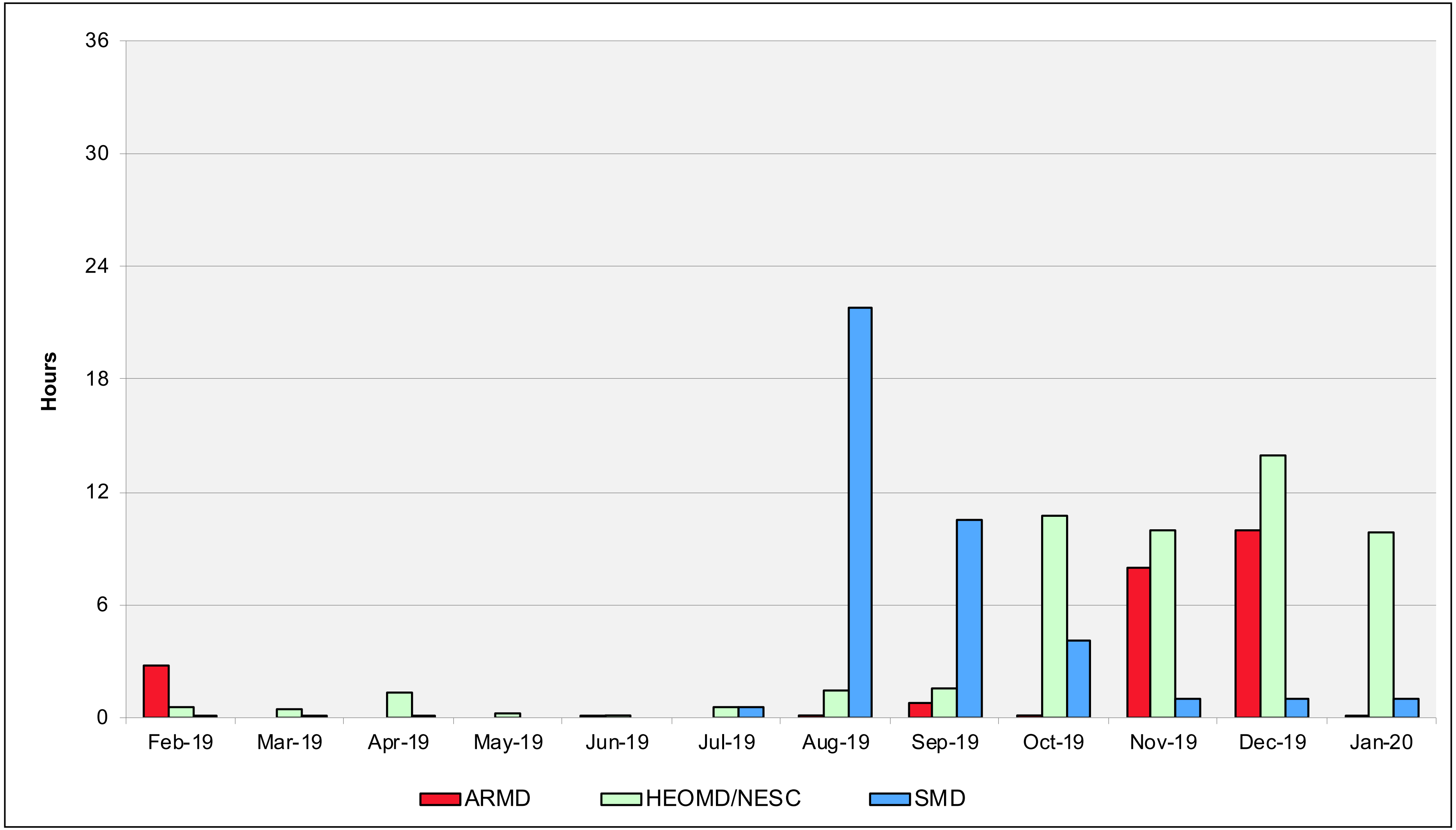
Merope: Monthly Utilization by Job Length



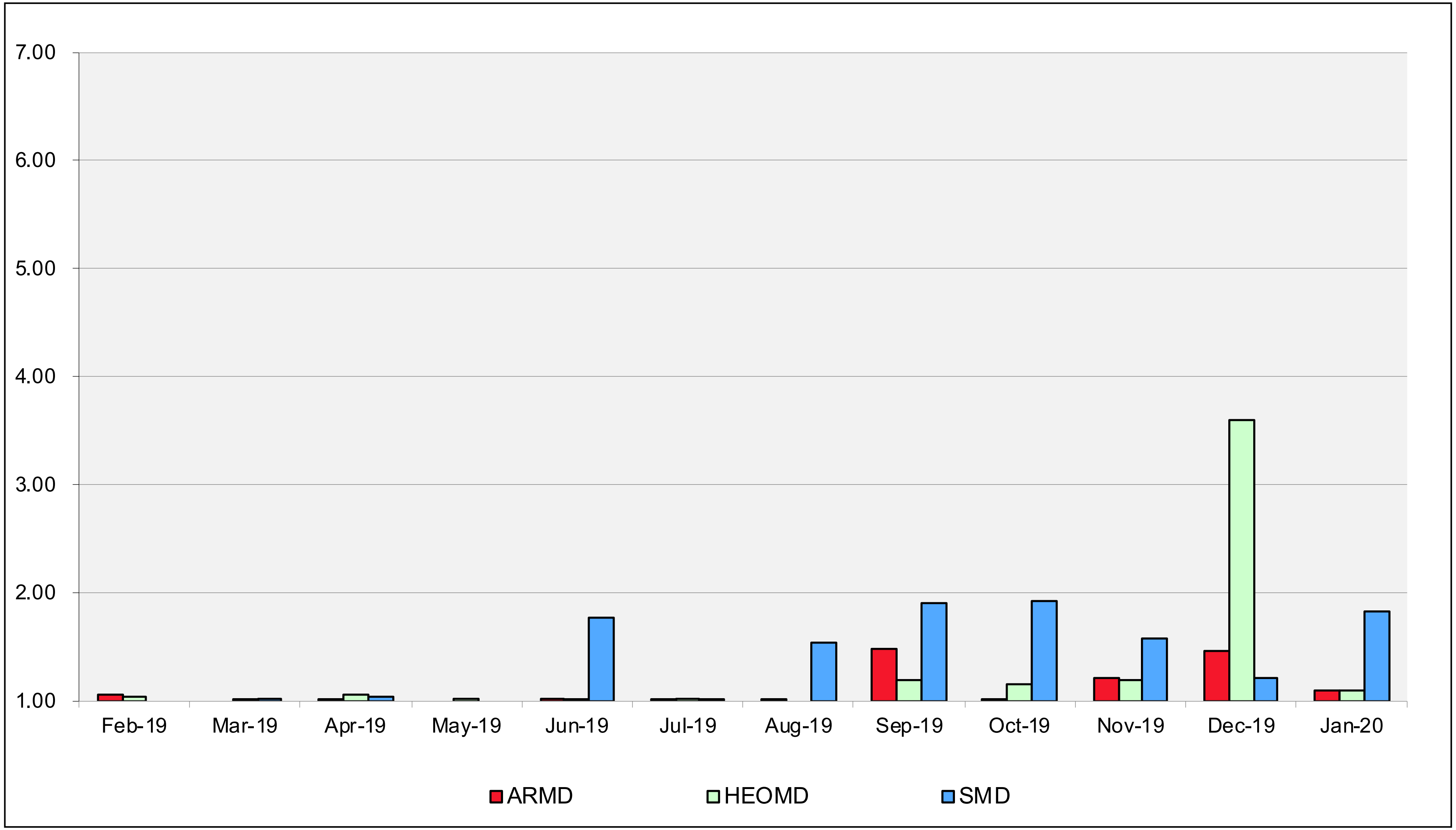
Merope: Monthly Utilization by Size and Length



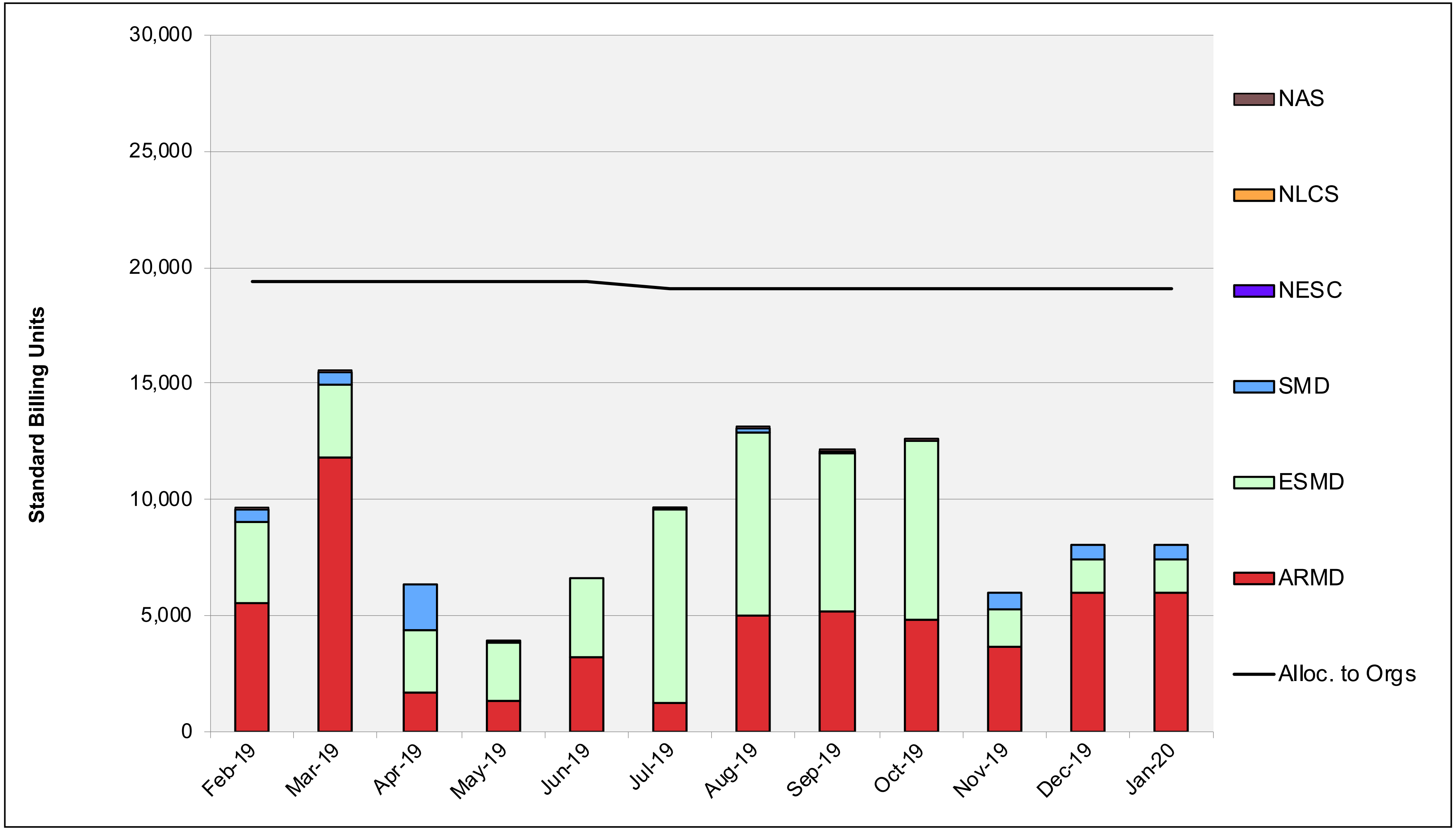
Merope: Average Time to Clear All Jobs



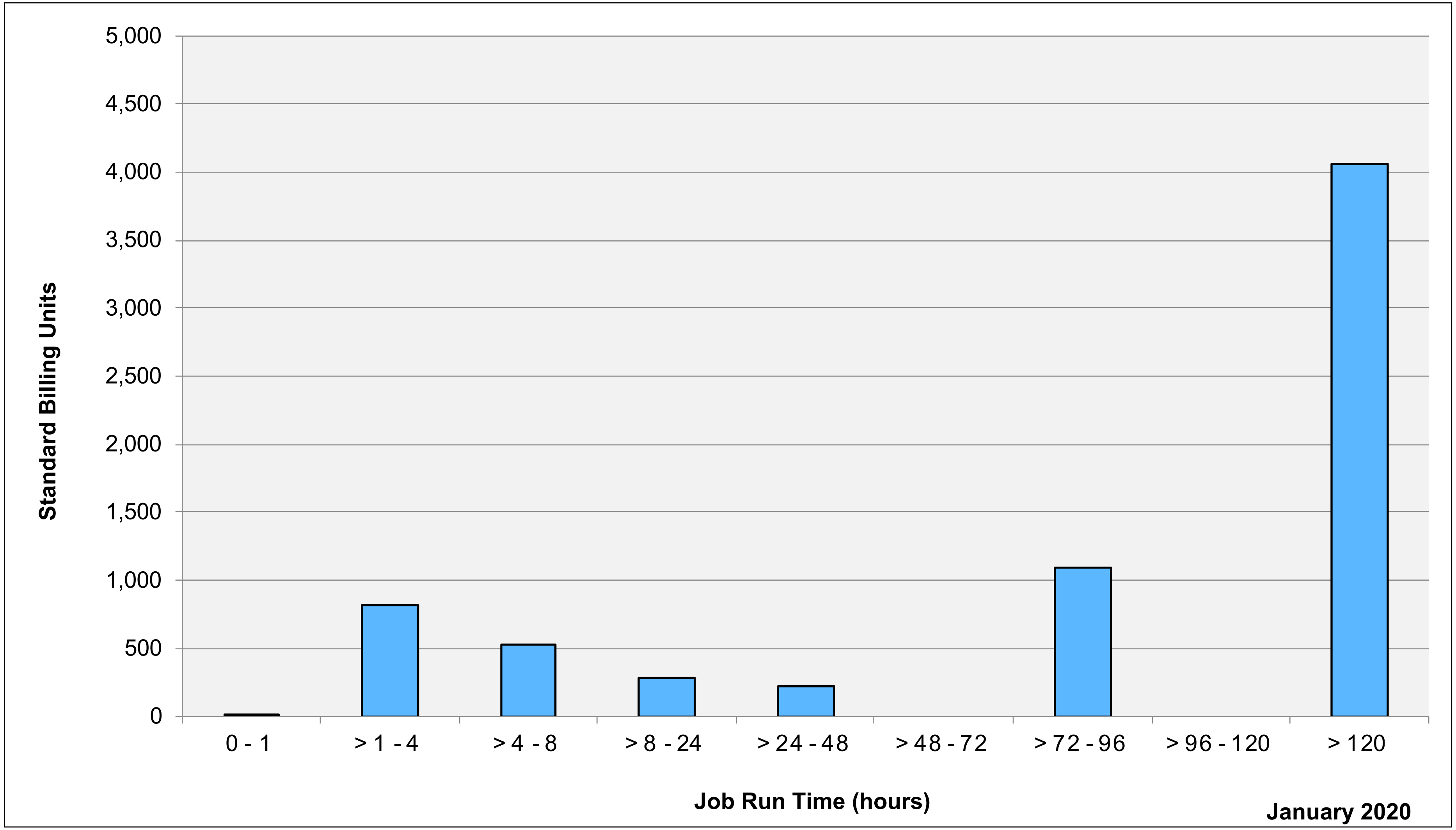
Merope: Average Expansion Factor



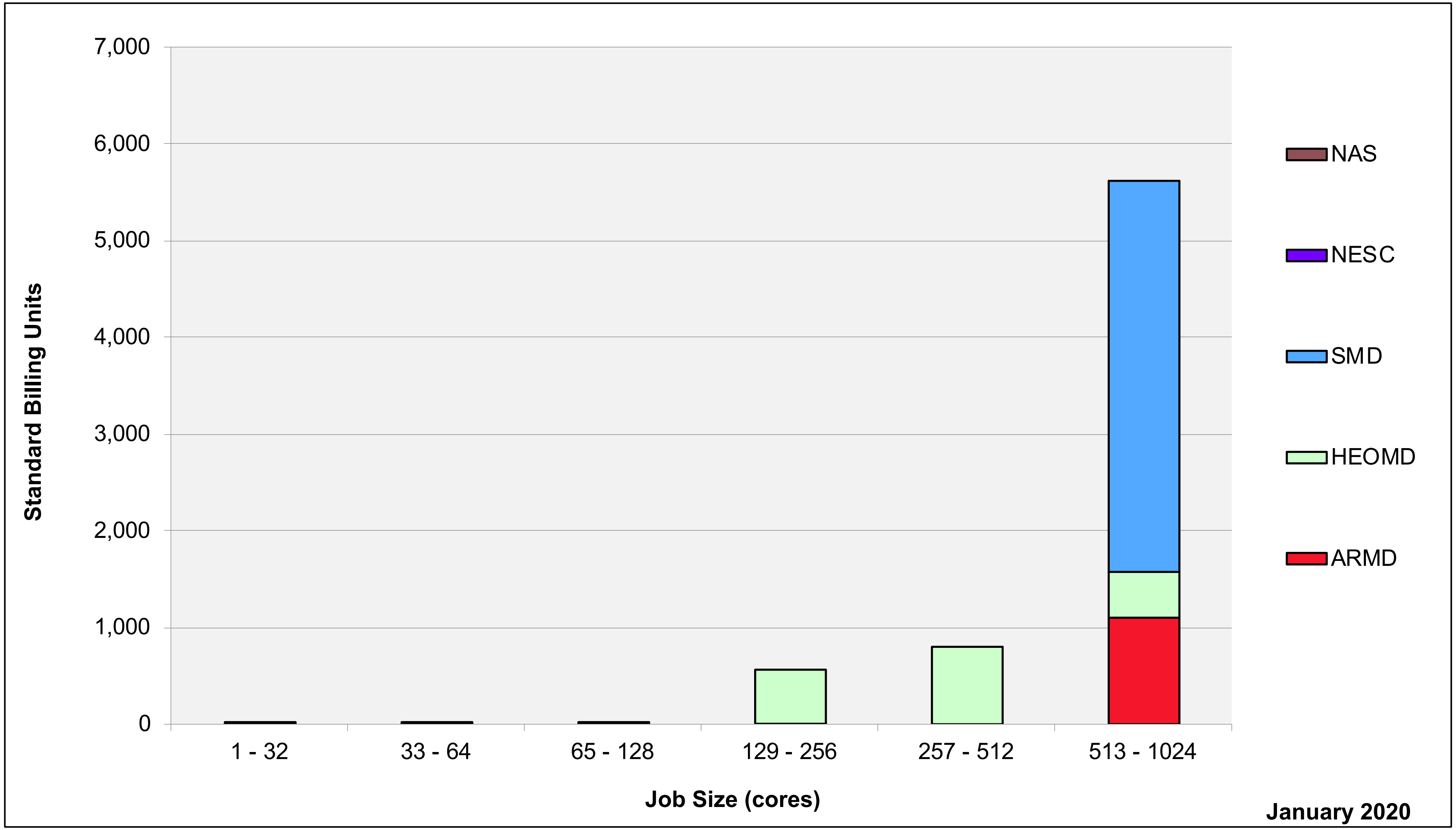
Endeavour: SBUs Reported, Normalized to 30-Day Month



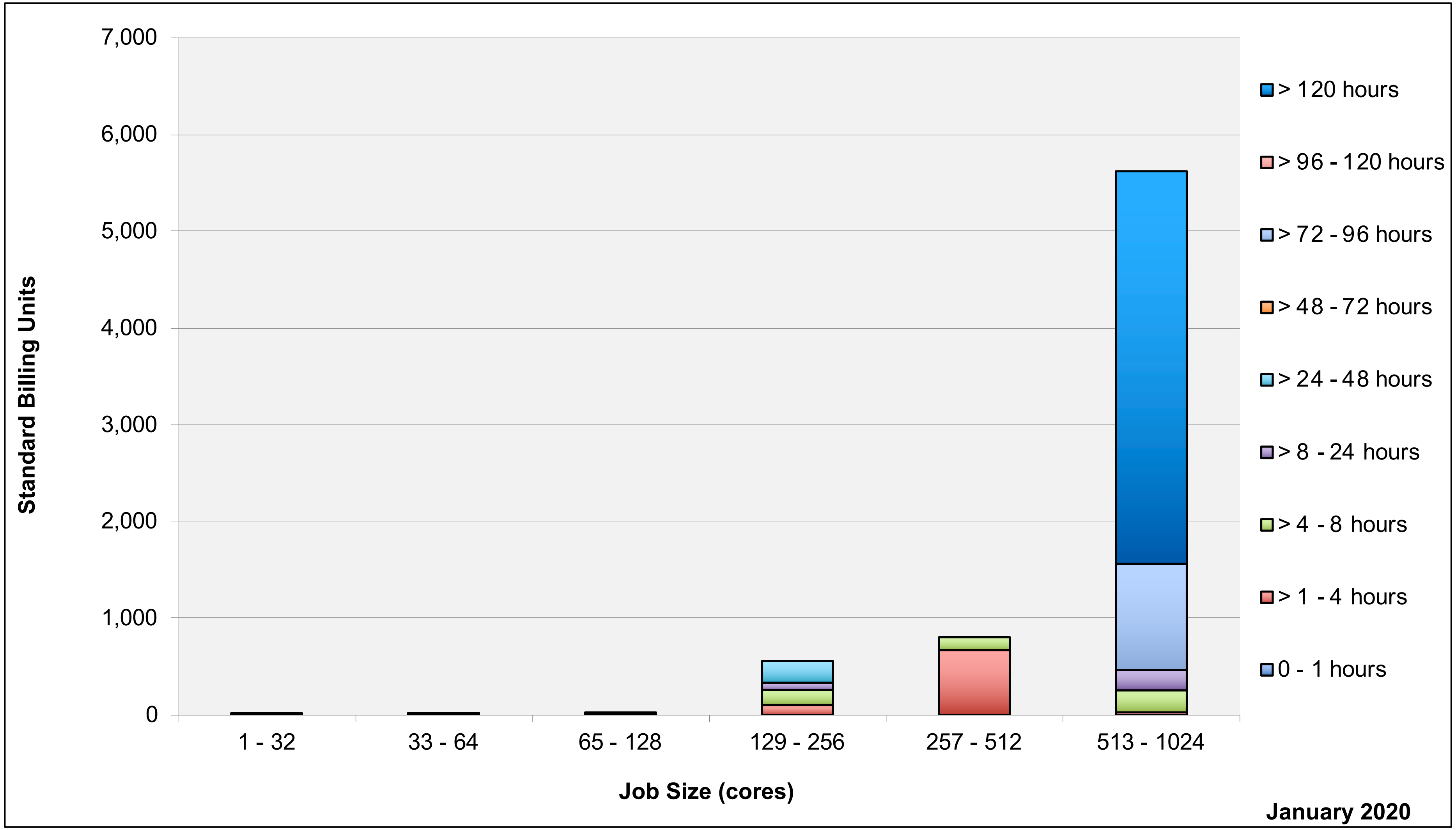
Endeavour: Monthly Utilization by Job Length



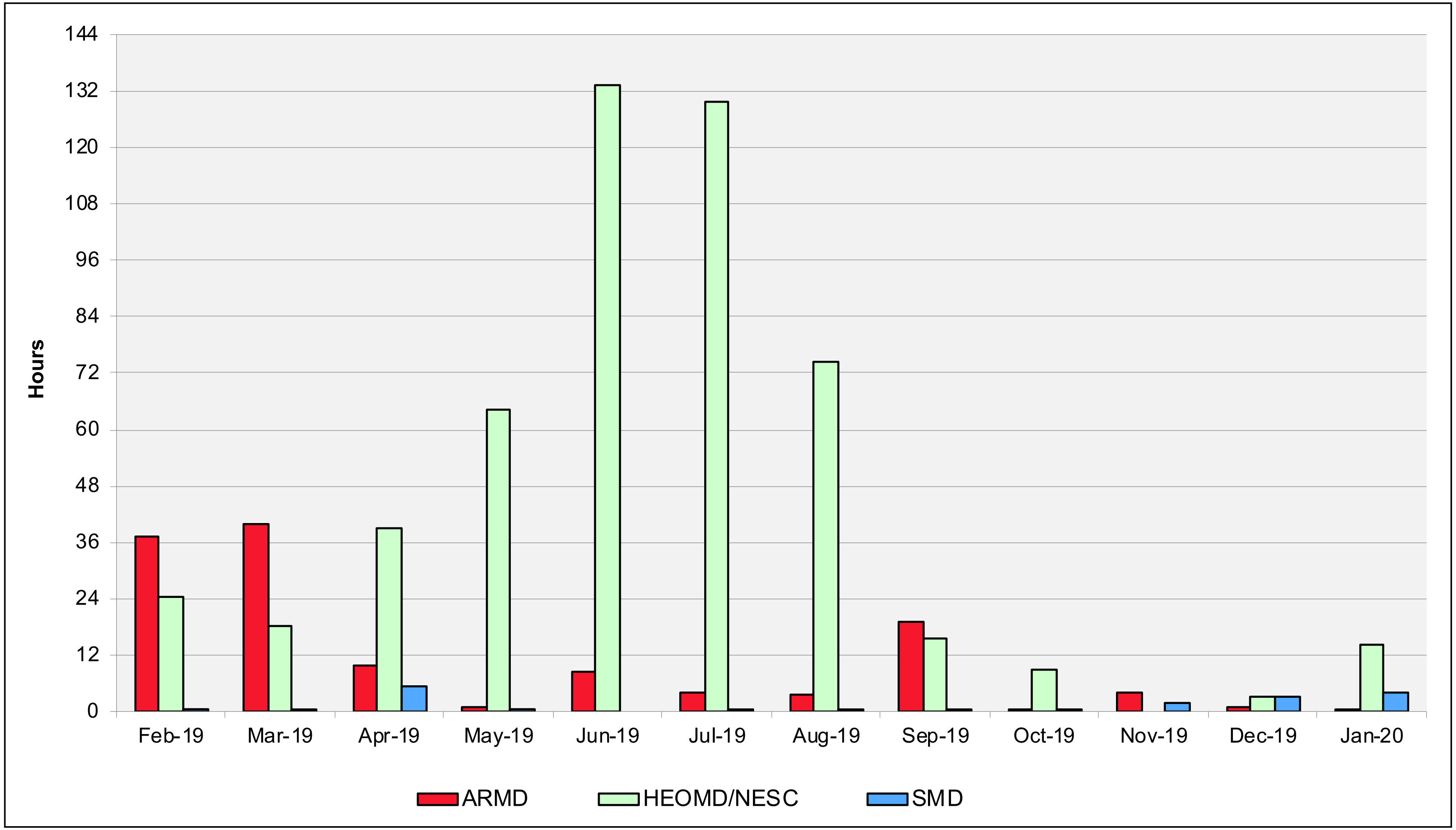
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor